A DATA-INPUT PROGRAM (MFI2K) FOR THE U.S. GEOLOGICAL SURVEY MODULAR GROUND-WATER MODEL (MODFLOW-2000)

Open-File Report 02-41

U.S. Department of the Interior
U.S. Geological Survey

A DATA-INPUT PROGRAM (MFI2K) FOR THE U.S. GEOLOGICAL SURVEY MODULAR GROUND-WATER MODEL (MODFLOW-2000)

By **ARLEN W. HARBAUGH**

U.S. GEOLOGICAL SURVEY

Open-File Report 02-41

Reston, Virginia
2002

U.S. DEPARTMENT OF THE INTERIOR
GALE A. NORTON, Secretary

U.S. GEOLOGICAL SURVEY
Charles G. Groat, Director

For additional information write to:

Office of Ground Water
U.S. Geological Survey
411 National Center
Reston, VA 20192
(703) 648-5001

Copies of this report can be can be purchased from:

U.S. Geological Survey
Branch of Information Services
Box 25286
Denver, CO 50225-0425

PREFACE

This report describes a computer program called MFI2K that can be used to prepare input data for the U.S. Geological Survey (USGS) ground-water model (MODFLOW-2000). The program has been tested in a variety of applications, but future applications might reveal errors that were not detected in the tests. Users are requested to notify the Office of Ground Water of the U.S. Geological Survey of any errors found in this user guide or the computer program at the address given on the back of the title page. Updates may be made to both the report and the program. Users can obtain the software and information about updates through the World-Wide Web pages for USGS software at http://water.usgs.gov/software/.

CONTENTS

FIGURES

A Data-Input Program (MFI2K) for the U.S. Geological Survey Modular Ground-Water Model (MODFLOW-2000)

by Arlen W. Harbaugh

Abstract

MFI2K is a data-input (entry) program for the U.S. Geological Survey modular three-dimensional finite-difference ground-water model, MODFLOW-2000. MFI2K runs on personal computers. MFI2K supports the solute transport and parameter-estimation capabilities that are incorporated in MODFLOW-2000. Data for MODPATH, a particle-tracking program for use with MODFLOW-2000, also can be entered using MFI2K. MFI2K is designed to be easy to use; data are entered interactively through a series of display screens. MFI2K also can be used in conjunction with other data-input programs so that the different parts of a model dataset can be entered using the most suitable program. MFI2K interfaces to an external program for entering or editing two-dimensional arrays and lists of stress data. This report provides instructions for using MFI2K.

INTRODUCTION

Computer models of ground-water flow require input data in order to define the simulated flow system. Most model programs read these data from one or more files rather than prompting for the data interactively. The reason for this result is partly evolutionary. When ground-water models were first developed in the 1960's, the primary focus was on developing the numerical methods to solve the differential equations of flow. The major challenge was being able to solve practical, real-world problems within the constraints of computer speed and memory. The simulations generally were small by present (2002) standards; therefore, preparing the data files using a card punch or text editor was easy. Further, computers of that time were not designed to allow for interactive input.

Presently, computers easily can handle large simulation problems where data preparation is a burdensome task. Considerable benefit can be obtained from an interactive program that helps prepare model-input data. The interactive program can prompt for the required data, check for errors, and ensure that files are created with the proper structure. Although adding interactive data entry into the model program would be possible, this addition is not desirable because the required memory and program complexity would be unnecessarily increased. Further, the wide variation in user preferences and needs makes it unlikely that any single method of interactive data input will meet all needs. Having data entry separate from the model is better so that different data-entry programs can be developed independently of the model program.

This report describes a data-input program, called MFI2K, for MODFLOW-2000, which is the U.S. Geological Survey (USGS) three-dimensional finite-difference ground-water model (Harbaugh and others, 2000). MFI2K includes support for the parameter-estimation (Hill and others, 2000) and solute-transport [originally documented by Konikow and others (1996) and subsequently updated for

MODFLOW-2000 (G.Z. Hornberger, U.S. Geological Survey, written commun., 2000)] capabilities that are incorporated in MODFLOW-2000. In addition, MFI2K can prepare data for MODPATH, which is a particle-tracking program that uses flows calculated by MODFLOW-2000 (Pollock, 1994).

MFI2K is based on the MFI program (Harbaugh, 1994), which is a data-input program for an earlier version of MODFLOW. In addition to supporting the newer version of MODFLOW, MFI2K has a more advanced user interface.

MFI2K users are assumed to be familiar with the design and input requirements of MODFLOW-2000. Users also must necessarily understand basic ground-water modeling concepts.

Design Goals

The primary design goals for MFI2K are listed below.

1. Easy to use—This goal is subjective. Some of the desired attributes are as follows: an intuitive user interface; the user is guided in a logical manner through the data entry process; and checking is done to make sure valid or reasonable data are entered.

2. Ability to use other data-entry programs with MFI2K—Modelers use a variety of computer applications to help manipulate their data. For example in the USGS, many modelers use geographic information system (GIS) software to store and manipulate data. It is important to be able to use data from the GIS along with data entered using MFI2K.

3. Low development cost.

4. Useful for a wide range of modeling problems from simple training exercises to large modeling projects.

5. Runs on personal computers.

Design Decisions

The following design decisions were made in order to fulfill the goals:

1. The programming language is Fortran—Many other languages would have been adequate for programming, but the author is most familiar with Fortran. Also, MODFLOW-2000 is written in Fortran; therefore, reading and writing data for MODFLOW is easy.

2. The Winteracter Subroutine Library (Interactive Software Services, 1998) is used as the tool for providing user interaction in MFI2K. Winteracter provides a set of tools for creating Fortran programs that interact with users through windows. Winteracter is sufficient for controlling the selection of options and entering miscellaneous data. It is insufficient for entry of large arrays (1,000 or more elements).

3. Spatial data will be entered into MFI2K using grid coordinates rather than arbitrary geographic coordinates that require transformation in order to determine grid coordinates. Also, data values for the grid must be entered into MFI2K for all locations required by MODFLOW-2000 as opposed to entering fewer values and having MFI2K interpolate the missing values. Transformation to grid coordinates and data interpolation capabilities could be obtained by using other programs along with MFI2K.

4. Large arrays of data and lists of point stress data will be entered through the use of an external program. Regardless of what interactive interface tool is used, writing a sophisticated user interface for entering arrays and lists of stresses is beyond the scope of this work. By interfacing with an available program, the greatest functionality can be obtained at the lowest cost.

5. As a further method of allowing the user to maximize the use of other software, MFI2K will allow external files to be specified as part of a MODFLOW-2000 dataset. These external files will not be read or modified by MFI2K, but the dataset will be setup so that MODFLOW-2000 will read these files. The use of external files in MFI2K is possible because MODFLOW-2000 allows arrays to be read from external files.

6. To avoid duplicate data, MFI2K will store all data in MODFLOW-2000 datasets rather than maintaining a separate database.

USER INSTRUCTIONS

MFI2K works by displaying screens to which the user responds. The user enters data, makes a choice, or reads displayed information. These user interactions are conducted using the keyboard and mouse as is typical in interactive programs on personal computers.

Entering Data with an External Editing Program

MFI2K uses an external editing program, such as a spreadsheet program, to allow the user to enter two types of data. The first type is array data. Most array data consist of data for a model layer; every cell in a layer has a value. In a spreadsheet program, the values are displayed and edited as a table; the cell locations are designated implicitly by the row and column locations in the table. If the data must be entered for multiple layers, it is treated as multiple layer arrays. One-dimensional arrays consisting of one row of data or one column of data are displayed and edited in a spreadsheet program as a one-row or one-column table.

The second type of data for which an external editing program is used is a list of data in which each entry includes a layer, row, and column grid location plus one or more data values that apply at that location. An example of this type of data is the list of wells for a particular stress period. Each well has four values, which are the three grid indices plus the well recharge rate (negative value indicates pumping). If MODPATH is being used, each entry also includes a code to indicate the cell face through which the stress is applied. The list values are displayed as a table in a spreadsheet program, with one line for each cell location.

The external editing program is run concurrently with MFI2K. When the external program is needed, MFI2K writes the data to be edited into a file named _mfiss.csv and displays a screen telling the user to activate the external program. The user must use the external program to read _mfiss.csv, edit the data, and save the data back into the same file. After the file has been closed within the external program, the user should select the OK pushbutton in the MFI2K screen, which will cause MFI2K to read the file to obtain the changed data.

Users commonly have two problems using this approach. The first problem is that a user immediately selects OK in the screen that says to use the external program rather than waiting until the data have been edited. The second common problem is that a user fails to close _mfiss.csv in the external program after saving the data. MFI2K will be unable to read the edited values from the file because the

file is still open in the external program. In this situation, MFI2K displays a screen telling the user to close the file in the external program.

MFI2K writes the file for external editing (_mfiss.csv) as a comma delimited text file, and the external program must write the data back into the file using a comma delimited structure. Excel and Lotus spreadsheet programs have been successfully used as external editing programs.

Running MFI2K

MFI2K resides on a personal computer as executable file mfi2k.exe. This file can be executed by using a Windows shortcut, using Windows Explorer, or entering the following command in a command window:

MFI2K
or
MFI2K *NameFile* ,

where *NameFile* is the MODFLOW name file.

If the name file is not entered as part of the command, then the first screen to appear will prompt for this. MFI2K only accepts name files that end with ".nam"; however, the ".nam" part of the name need not be entered because MFI2K will automatically add it, if necessary. The part of the file name before ".nam" is called the dataset name, and this can be from 1 to 28 characters.

The dataset name is used as the prefix for the names of many files that MFI2K creates. These file names are constructed by adding a period plus 2 or 3 characters to the dataset name. Some examples are:

.log is the suffix for a log file of information generated by MFI2K;
.ba6 is the suffix for the Basic Package file of MODFLOW-2000;
.bc6 is the suffix for the BCF Package file of MODFLOW-2000;
.mpn is the suffix for the MODPATH name file;
.mp is the suffix for the main MODPATH data file.

The dataset name cannot include characters that are invalid as part of a file name on the particular computer and operating system being used.

If a name file exists, it is read along with all of the MODFLOW input data, and the Main Menu is displayed. If a name file is new, the next screen prompts for confirmation that it is acceptable to create a new model dataset. If it is not acceptable to create a new dataset, MFI2K stops without performing other tasks. MFI2K stops at this point because it is assumed that the user intended to enter the name of an existing dataset. The user then can restart MFI2K. If it is permitted to create a new dataset, the next screen prompts for the number of layers, rows, and columns. These grid size values cannot be changed within MFI2K after this screen is accepted; therefore, be careful to specify them properly. This screen also allows the choice to be made between free and fixed format. This refers to the structure of MODFLOW data files. Free format means that the width of each data field can vary, whereas fixed format means that the field width for each value is fixed. This option applies only to those packages that support both formats.

Main Menu

Once the dataset name is established, a window is created that includes the Main Menu at the top and information about the active simulation options as shown in figure 1. Most of the menu items control data entry; however, the "FILE" item provides typical functions for saving data and exiting the program, and the "OPTIONS" item provides useful information, such as file names of all files that will be used in the MODFLOW-2000 simulation.

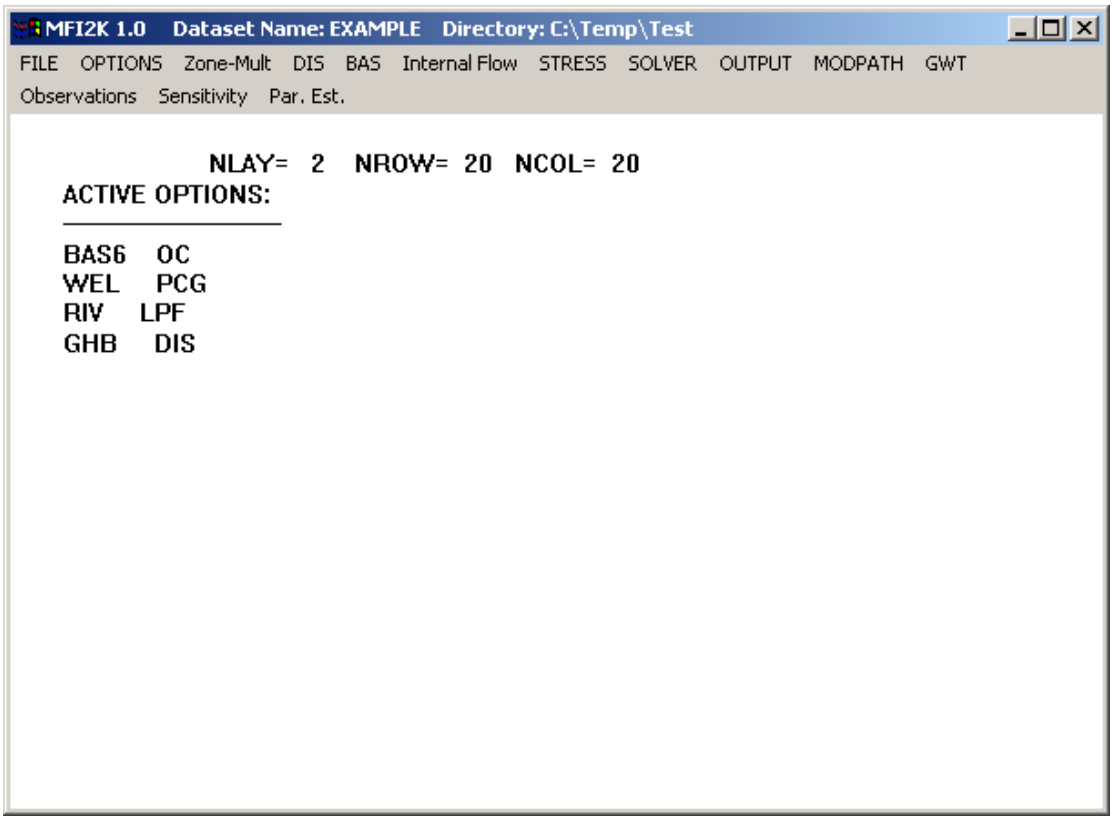

Figure 1. Main Menu for data-input program MFI2K.

The data-editing menu items generally are organized according to MODFLOW's files. For example, the "Zone-Mult" item allows entry of data in the files that specify zone and multiplier arrays. The "DIS" item allows entry of data for the discretization file. To keep the number of choices in the Main Menu from growing too large, many of the menu items have sub menus. For example, the "Internal Flow" item contains items that allow entry of data for the Block-Centered Flow and Layer-Property Flow (LPF) Package files. The stress packages are combined into a single menu item, "STRESS." The solvers for which MFI2K can prepare data are included in the single "SOLVER" item. "MODPATH" also is a menu item, which allows entry of data needed for MODPATH's Main Data file.

FILE Menu Item

Selecting the "FILE" menu item causes a submenu to be displayed with these items: "Save As", "Save", "Run MF2K", "Abort", and "Exit (and Save)." The "Save As" item saves the dataset using a new dataset name, including the name file. All listing files, package files, option files, and process files are renamed. The "Save" item saves the dataset using the current name. The "Run MF2K" item saves data using the current name and runs a program named MFI2KRUN.BAT. This BAT file is intended to include commands to cause MODFLOW-2000 to run. The "Abort" item exits MFI2K without saving data. The "Exit (and Save)" item saves data and then exits.

OPTIONS Menu Item

Selecting the "OPTIONS" menu item causes a submenu to be displayed with these items: "Check Complete", "Deactivate", "Show Files", and "GLOBAL/LIST Files". The "Check Complete" item shows whether or not each active option has all of its data defined. If an option is designated as "incomplete," then some of its data have not been specified. The specific undefined data can be displayed for an option by selecting the appropriate editing item from the Main menu. For example, if Block-Centered Flow (BCF) data are incomplete, select BCF from the "Internal Flow" submenu. This selection will cause a BCF dialog to appear that includes a "Check Data" option. Selecting that option will display all undefined data for the BCF Package. The user may be surprised that some data that have not been entered do not show as undefined. This occurs because MFI2K automatically specifies defaults for many values. These values can be changed if desired, but they need not be explicitly defined by the user if the defaults are adequate. The "Deactivate" item allows simulation options to be turned off. The "Show Files" item displays all files that have been defined and shows their use. "The GLOBAL/LIST Files" item allows the names of the Global and List files for the simulation to be specified.

The "Deactivate" item is provided because the data editing menus do not provide a mechanism for turning off options. Once data entry is initiated for any MODFLOW option, then MFI2K activates that option and will write data files for that option when data are saved. When MODFLOW runs, that option will be invoked. Likewise, if data entry for MODPATH is initiated, then MODPATH data files will be written. If an option is deactivated, the data for that option will no longer be saved whenever MFI2K saves data. Also, MODFLOW and MODPATH will not include that option when they subsequently are executed. However, if a file for a deactivated option was present prior to its deactivation, that file will still be present after MFI2K exits.

Data Editing Menu Items

Selecting a data editing menu item invokes a corresponding dialog screen called a primary dialog. Most primary dialogs consist of a list of options that activate other dialog screens for the actual data entry. The primary dialogs that can activate additional screens have a CLOSE option, which will return to the Main Menu. The user must ultimately end up back in the Main Menu in order to exit MFI2K. Some of the primary dialogs include a "Check" item, which displays information about undefined data.

Entering Two-Dimensional Arrays

There are three methods that can be used to define two-dimensional arrays in MFI2K. These correspond to the three methods that MODFLOW and MODPATH use for defining arrays. The first method, referred to as the Constant Method, is to make the entire array a constant.

The second method, called the Package Method, is to define individual values for each array element that MFI2K writes into the appropriate MODFLOW file. This file typically is a package file, which is the reason for calling this the Package Method; however, data also are written into other files as appropriate such as process or MODPATH files. When the Package Method is used, the user enters the values for the individual array elements using an external data-editing program. (See the Entering Data with an External Editing Program Section above.) MFI2K writes the array-element values in the appropriate MODFLOW file when exited. After an array is first designated as being defined by the Package Method, MFI2K activates the external editing mechanism to allow the array elements to be entered. Once an array initially has been defined using the Package Method, its elements can be examined or modified using the external editing program. The "Send for External Editing" pushbutton activates the external editing mechanism.

The third method, called the Separate Method, is to specify that the values for individual array elements are in a separate file that MFI2K does not read or write. Although MFI2K does not actually

read or write the contents of such files, MFI2K incorporates information about these files into the proper locations in the dataset so that MODFLOW and MODPATH will read them. The files must be prepared using other software.

All three methods of defining arrays are specified through the same screen. An example screen that defines an array is shown in figure 2. In this example, the Constant Method is being used. The other two methods can be selected by clicking on the appropriate option (called a radio button). Notice that for each method there are different data fields that can be specified. The fields for a method cannot be modified unless the method first is selected. For the Package and Separate Methods, a constant is specified that is multiplied with each element of the array to make the final value. Thus, the entire array can be rescaled by changing the multiplier. Note that the array multiplier is different from a multiplier array, which is used for defining parameters.

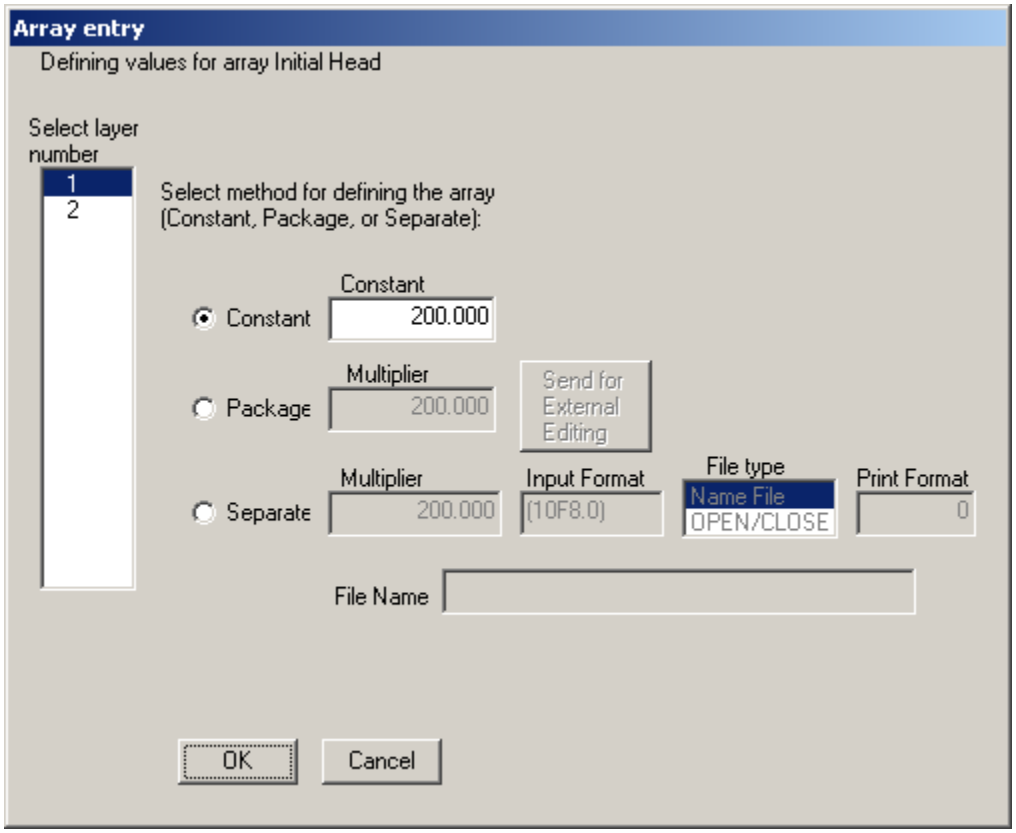

Figure 2. Example screen showing methods of array definition in MFI2K.

For arrays defined using the Separate Method, the information that will allow MODFLOW or MODPATH to read the array must be specified. This information includes the file name, an input format, and a code for which format to use when printing the array after it is read. Remember that MFI2K does not read values for these arrays; therefore, if errors occur, such as an incorrect format or an invalid file name, they will not be detected by MFI2K. Such errors will not be detected until MODFLOW or MODPATH is executed. Choose a file type, which can be either "OPEN/CLOSE" or "Name File". This choice corresponds to the capability of MODFLOW to declare the name of a data file in either the array control record or the MODFLOW name file (Harbaugh and others, 2000, p. 86). If a file is used to define a single array, then either file type can be used. If a file is used for more than one array, then the file type must be the same for all the arrays, and it is important to specify the proper file type. If the identical data are to be specified for all of the arrays defined by the file, then the file type should be "OPEN/CLOSE". For this file type, the same file will be reopened each time it is used to define an array, which causes the same data to be read over and over. If the same file contains multiple arrays, each of which may have

different values, then the file type must be “Name File”. This type of file is left open as each array is read so that the multiple arrays are read in sequence from the file.

Entering One-Dimensional Arrays

One-dimensional arrays are defined in the same ways as two-dimensional arrays. That is, the same three methods, Constant, Package, and Separate, can be selected. Although the amount of data to be entered is less than for a two-dimensional array, the input methods function the same. When using the Package Method, the data to be edited in the external editing program will show up as either a row or column depending on the type of data. For example, the grid spacing along a row (DELR) shows up as one row in the external program, with one value for each column in the model grid. Similarly, column (DELC) values show up as one column in the external program with one value for each row in the model grid.

Entering List Data

“List data” refers to data that are specified in a MODFLOW file for a group of cells using one line of data for each cell. A line of data includes the layer, row, and column indices for one cell plus some additional information. For example, list data are used to define wells and river reaches. In MFI2K, four methods can be used to define list data: None, Previous, Package, and Separate. The None Method indicates that the list has no entries. The Previous Method indicates that the list from the previous stress period should be reused. This method is not available for the first stress period. The Package and Separate Methods are similar to the methods of the same name for arrays. The Package method allows the list of data to be edited using the external editing program. (See the Entering Data with an External Editing Program Section above.) In the external editing program, the list shows up as a table with one row for each cell in the list. The first two lines of the table contain labels for the columns. These two lines of the table should not be modified when editing the data. The options for defining list data are shown on the right side of figure 3.

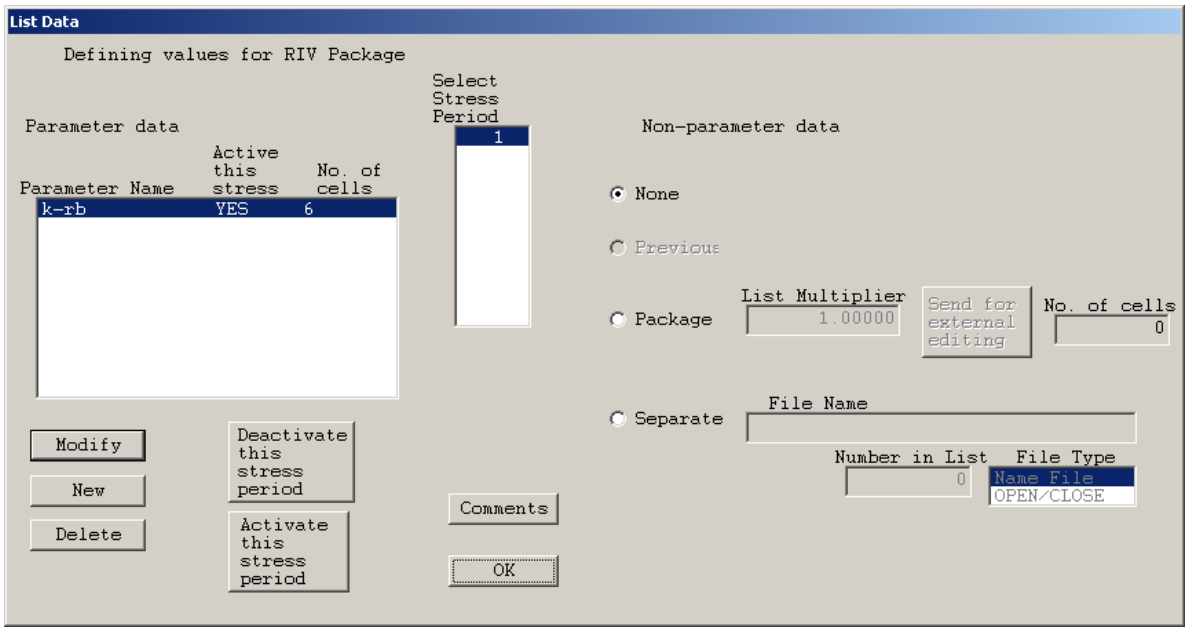

Figure 3. Example screen showing options for defining list data in MFI2K.

Entering Parameters

Parameters provide a mechanism for defining input data that apply to many cells. A parameter is a single value that can be used to determine data values for multiple cells. Parameters often can make data input more convenient because of the multi-cell capability. By changing a single parameter value, the input data will be changed for all the associated cells. Also, input data must be defined using parameters

in order to make use of parameter estimation. MFI2K allows parameters to be defined for all the types of data for which parameters can be used in MODFLOW-2000.

The possibility for using parameters to define list data is shown on the left side of figure 3. List parameters can be used simultaneously with nonparameter lists. A list parameter is first created using the "New" pushbutton. A new list parameter is an empty list. Values can be added to the list using the "Modify" pushbutton. When modifying a list parameter, the Package and Separate options can be used to specify the list. A list parameter can be active or inactive in any stress period, and this is controlled by the "Deactivate this stress period" and "Activate this stress period." A common error is to create a parameter and not activate it in appropriate stress periods. List parameters can be deleted using the "Delete" pushbutton

A screen for defining arrays for the LPF Package is shown in figure 4. The right side shows that the arrays can be defined without using parameters. The "Select Array" list shows the arrays that can be defined for the layer selected in the "Select layer" list. In this example, four array types can be defined for layer 1. These arrays can also be defined using parameters, which is controlled by the left side of the screen. For any array type, all layers must be defined entirely with or without parameters. That is, parameters and nonparameters cannot be used to define the same array type. Once a parameter is defined that corresponds to an array type, MFI2K removes that array type from the "Select array" list of nonparameter arrays. Then, it is the user's responsibility to insure that the defined parameters define data values for all cells for all layers for which that data type are required.

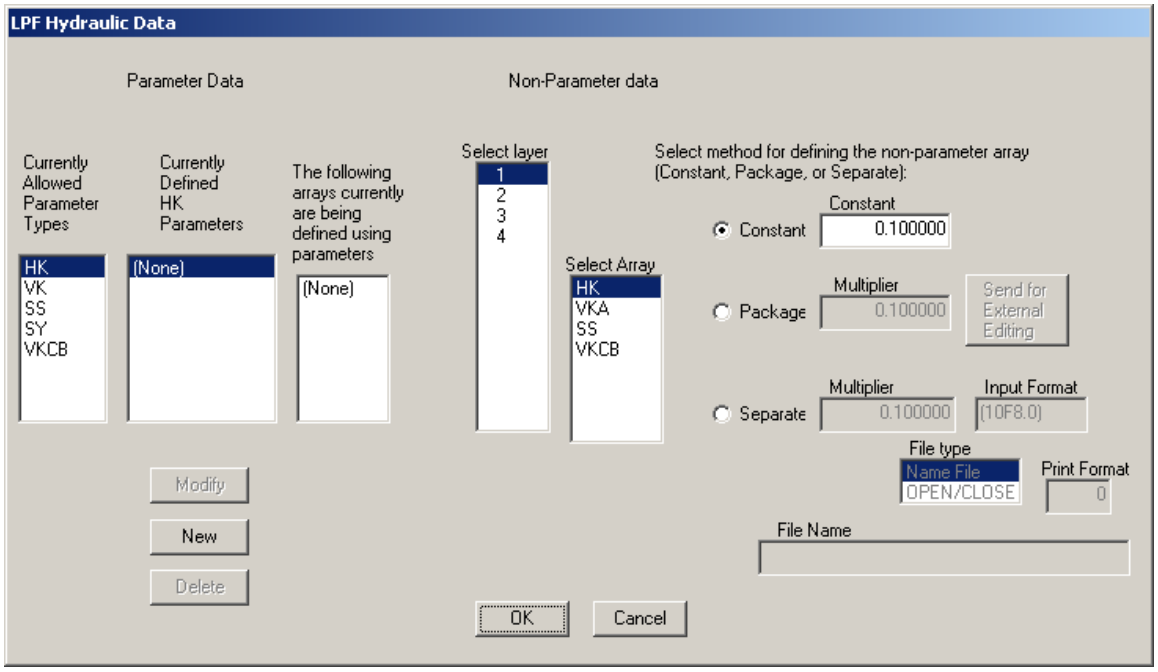

Figure 4. Example screen showing array definition in MFI2K.

To define an array parameter, select the parameter type from the "Currently allowed Parameter Types" list. The "New" pushbutton creates a new parameter. This selection will cause the screen shown in figure 5 to appear. Each line in the table defines an array cluster, which defines values for all or part of the cells in one layer. The use of array clusters is defined in Harbaugh and others (2000, p. 14 and p. 61). In order to use a multiplier array other than "NONE" or a zone array other than "ALL," these arrays must be defined. These arrays can be defined using the Zone-Mult Main Menu item or the "Edit Multiplier Arrays" and "Edit Zone Arrays" pushbuttons (fig. 5). When a zone array is used, 1 to 10 zone values must be specified in fields Z1 through Z10. If less than 10 zone values are used, the fields must be filled starting with Z1; and there must not be any blank fields between nonblank fields.

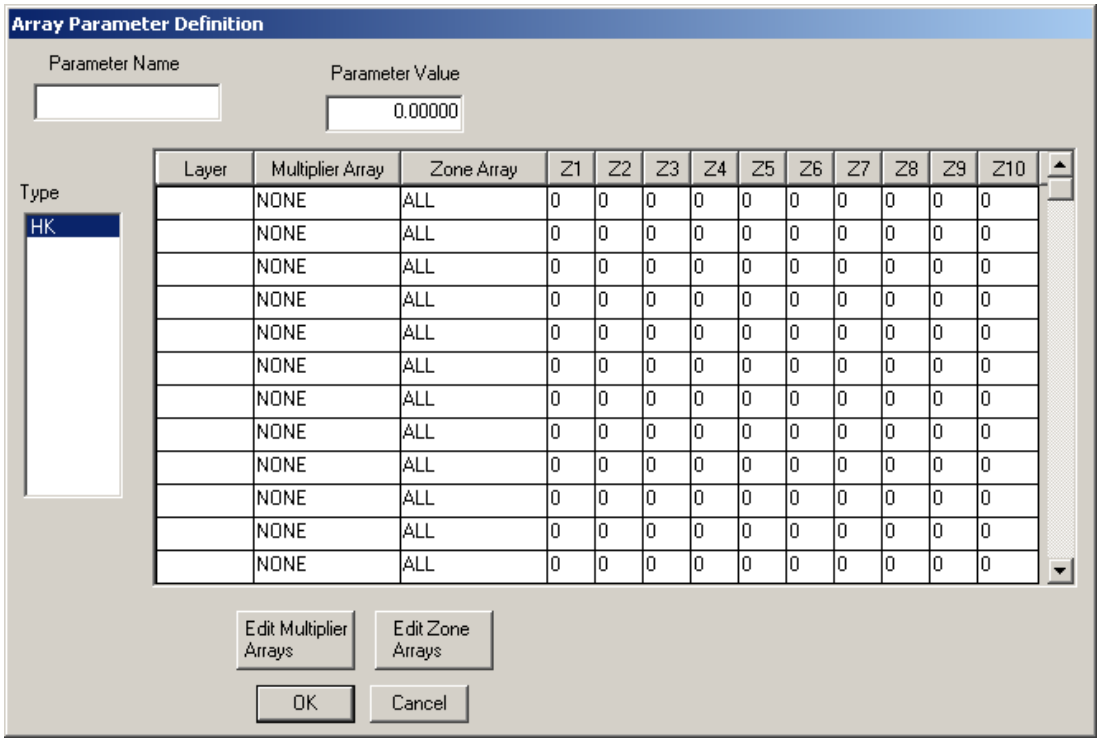

Figure 5. Example screen showing definition of array parameters in MFI2K.

The "Modify" pushbutton in the array definition screen (fig. 4) allows an existing parameter to be modified using the array parameter screen (fig. 5). The "The following arrays currently are being defined using parameters" list shows all array types that are being defined using parameters. To revert to defining an array type without using parameters, use the "Delete" pushbutton to delete all parameters of that type. The array type then will appear in the nonparameter data section of the screen in the "Select array" list.

For LPF, the parameter types are the same as the array types, except for the VKA array. Parameters that define the VKA array are designated as VK or VANI depending on the value of the LAYVKA flags for each layer. The user must define appropriate parameter types to define VKA as specified by the LAYVKA flags (see Harbaugh and others, 2000, p. 61).

OK and Cancel Pushbuttons

As is typical in interactive programs, "OK" and "Cancel" pushbuttons are included in many of the MFI2K screens. Both buttons cause the screen to be terminated, but the "Cancel" button causes data changes to be ignored, whereas "OK" causes changes to be accepted. However, the function of the "Cancel" button on MFI2K is limited on many of the screens because some of the screen selections other than the "OK" pushbutton cause the current data to be accepted. Once acceptance happens, "Cancel" can no longer prevent that data from being accepted. This action is easiest to explain by example. The screen that allows initial head to be specified (for the BAS Package) is shown in figure 2. In this example, the model consists of two layers. The screen contains a layer field, and the layer that currently is being defined is highlighted (layer 1 in fig. 2). In order to define data for a different layer, the desired layer can be selected. Changing the layer does not cause the screen to terminate but causes the data for the previous layer to be accepted. Thus, if the user changed from layer 1 to layer 2, the layer 1 data would be accepted. Thus, entering "Cancel" after changing to layer 2 would not prevent the changes that had been made to layer 1 from being accepted. Other screens allow more than one array to be defined as well as more than one layer. In these screens, changing the array also causes the current array to be accepted for the current layer.

Obtaining Help When Using MFI2K

For ease in identifying the specific data variables being entered, the MFI2K data screens contain brief definitions of the variables being defined or specify the variable names (or both). If this minimal information is inadequate, then the MODFLOW-2000 (Harbaugh and others, 2000; Hill and others, 2000) or MODPATH (Pollock, 1994, appendix A) documentation should be consulted for a more complete description of the data variables.

Further, the appendix contains help information for each screen. The information is organized similar to the MFI2K Main Menu. This appendix will be distributed as a separate file with the MFI2K software (see the report preface) so that the help information can be examined interactively while MFI2K is running.

Data Recovery if MFI2K Aborts

If something goes wrong and MFI2K aborts, some data may be recoverable. If the error is detected by MFI2K, MFI2K attempts to save all current data in files named "MFI" followed by a period and a two- or three-character option designation; for example, "MFI.RCH" for the recharge option. Even if MFI2K aborts without detecting the cause—for example, the power to the computer could be shut off—there may be some recoverable data. This occurs because every time the menu for editing data for a primary option is completed through the "DONE" option, a backup file of the data for that option is written to an "MFI..." file. However, the user would have to use a text-editing program and have knowledge of the structure of the files (from MODFLOW-2000 or MODPATH documentation) in order to extract data from them.

Running MODFLOW and MODPATH

MFI2K creates a complete dataset for running MODFLOW-2000 and MODPATH except for the data files for arrays and lists that are specified using the Separate Method. The MODFLOW-2000 name file is *fname*.nam, where *fname* is the dataset name. If MODPATH is being used, MFI2K also creates the MODPATH name file, and its name is *fname*.mpn.

Although MFI2K creates datasets of the proper form for MODFLOW-2000 and MODPATH, incorrect data may possibly be entered using MFI2K. MFI2K does some data checking in order to reduce the chance for errors, but the checking is not exhaustive. Further, no amount of checking can detect data-entry errors in which a reasonable, but incorrect, value is entered mistakenly. Some errors will cause MODFLOW-2000 or MODPATH to stop before completion, whereas others will result in what might first appear to be normal execution, but the results are wrong. Thus, the output files from MODFLOW-2000 and MODPATH always should be examined to make sure that data have been defined as intended.

Miscellaneous Details About Using MFI2K

Input Data that MFI2K Generates

Users already familiar with MODFLOW-2000 and MODPATH or who carefully examine the MODFLOW-2000 and MODPATH input instructions will notice that the MFI2K data screens do not directly include all data variables required for MODFLOW-2000 and MODPATH. This is because MFI2K generates some variables either by assumption or from other requested information. For example, the number of river reaches is determined by the number of nonblank lines in the list of river reaches specified in the file that is saved by the external editing program. File units are generated automatically.

Input Data Shared Between MODFLOW and MODPATH

Some variables are shared between MODFLOW and MODPATH. In MFI2K, these shared variables are entered only within MODFLOW data-editing screens. That is, the shared variables are not included as part of the screens used for MODPATH data. These shared variables are:

HNOFLO
HDRY
LAYCON (BCF Package) or LAYTYP (LPF Package)

Note that IBOUND is not shared by MODPATH and MODFLOW, although both MODFLOW and MODPATH have an input variable named IBOUND. The reason is that MODPATH makes expanded use of IBOUND. In addition to indicating boundary conditions as in MODFLOW, MODPATH uses IBOUND to indicate zones for the purpose of controlling which particles and pathlines are displayed and their colors. There are situations in which different IBOUND values may be desired for MODFLOW and MODPATH. Thus, these are viewed as different arrays, except that when MODPATH is first activated, any MODFLOW IBOUND arrays that are constant or package arrays are copied to the IBOUND for MODPATH. Further, whenever IBOUND is modified in MODFLOW or MODPATH, the values are checked for consistency (no- flow, constant-head, and variable-head cells at the same locations). If there are inconsistencies, the user is notified, but nothing is done to attempt to remedy the inconsistencies. No consistency checking is done for any layers for which IBOUND is defined using the Separate Method in either MODFLOW or MODPATH.

MODPATH includes the capability to specify which cell face receives a particular stress. This capability is incorporated in MFI2K through the screens in which stress data are entered. When MODPATH is active, the stress screens include the capability to indicate the cell face for the stress. For the River, Well, Drain, and General-head Boundary stresses, the stress face is specified in the list of stresses each stress period. For Recharge and Evapotranspiration stresses, the face is specified as a single value for all cells for the entire simulation. Thus, activating MODPATH prior to entering stress data is more efficient if the user knows that MODPATH eventually will be used. This specification will allow the stress faces to be entered when the other stress data are entered. If stress data are entered prior to activating MODPATH, then the stress screens will need to be reentered after MODPATH is activated if there is a need to specify specific faces to receive stresses.

Note that for the IFACE data to be conveyed from MODFLOW-2000 to MODPATH, the COMPACT BUDGET option must be specified in the "Output Files and Formats" screen that is accessed through the "Output" Main Menu item.

Constraints in MFI2K that are not in MODFLOW-2000 and MODPATH

Ideally, MFI2K should impose no constraints on data that MODFLOW-2000 and MODPATH do not impose; however, some compromises were made to minimize development effort. Additional constraints imposed by MFI2K are listed below. Some configurable limits were set in the program, which relate to the amount of memory used by MFI2K, that are not included in this list of constraints.

1. The precision of data values in files created by MFI2K is controlled by MFI2K. In most cases, values will be written with at least four significant digits. If the precision used is inadequate, MFI2K cannot be used or must be modified to be more precise.

2. If output does not occur at regular intervals (every time step, end of every stress period, or end of simulation), then a maximum of 47 times can be entered at which output will occur.

3. If specific layers for printing or saving head or drawdown are listed rather than using the default of having this information output for all layers, a maximum of 15 layers can be specified.

4. A maximum of 92 file units can be used for MODFLOW files—units 1-4 and 7-94. A maximum of 77 file units can be used for MODPATH files—units 1-4 and 7-79.

Using MFI2K with a Dataset not Originally Created by MFI2K

MFI2K can work with MODFLOW-2000 and MODPATH files that were not created originally using MFI2K. The main constraint is that the name files must end in .nam and .mpn, respectively. Also, note that MFI2K will not rewrite the data in the same format as previously used. Thus, some precision of values may be lost.

Using MFI2K When MODFLOW-2000 Includes Capabilities that MFI2K Does Not Include

MODFLOW-2000 is designed to be enhanced, and accordingly, MFI2K generally will not be up-to-date with MODFLOW-2000. If a user is using parts of MODFLOW-2000 that are not supported by MFI2K, the program still can be used for those parts that MFI2K does support. Files for packages not supported by MFI2K must be prepared by other means, and the names of these files must be added manually to the name file. If MFI2K does not support a file type that is included in the name file, MFI2K will leave the line containing the unknown file type in the name file.

PROGRAM DOCUMENTATION

The source code for MFI2K is not included in this report; the code can be obtained as described in the report preface. The information in this section is provided for the purpose of helping the user modify the source code if needed.

Memory Usage

MFI2K stores in memory the data that are read. MFI2K uses a single array, X, to store most of its data. Locations of variables within X are maintained by MFI2K. MFI2K maintains a list of variable names and their locations within X. The list is searched whenever the location of a variable is needed.

Lists of stress data for a stress period require special consideration because MFI2K does not require the maximum size of a list to be specified. MFI2K allows the user to enter list data of varying length, and the length can change at any time. In order to store lists of varying size, MFI2K allocates memory for lists in blocks. Each block has a fixed size, but a list can consist of up to 10 blocks.

The following variables control how much memory MFI2K can use. These variables are defined in the file "mfi2k.inc," which is an include file used in many of MFI2K's subroutines. In addition to the size of the X array, these variables specify the size of a number of other arrays used by MFI2K to keep track of data.

LENX—Number of elements in the X array
MXVAR—Maximum number of variables
MXARR—Maximum number of variables that are arrays
MXFNAM—Maximum number of files
MXLIST—The number of entries in a list block; a list can consist of up to 10 blocks

Portability

Although MFI2K is written in Fortran, which has been widely implemented on many kinds of computers, MFI2K is strongly dependent on the Winteracter Subroutine Library (Interactive Software Services, 1998). Winteracter is a commercial product that is not as widely available as Fortran. Calls to Winteracter subroutines are dispersed throughout the parts of the program that interact with users.

MODFLOW-2000 Capabilities Supported by MFI2K

The following list shows the capabilities of MODFLOW-2000 that are included in MFI2K.

Discretization file
Basic Package
Block-Centered Flow Package
Layer-Property Flow Package
Well Package
Drain Package
River Package
Evapotranspiration Package
General-Head Boundary Package
Recharge Package
Strongly Implicit Procedure Package
Slice-Successive Overrelaxation Package
Preconditioned Conjugate Gradient Package (Hill, 1990)
Direct Solution Package (Harbaugh, 1995)
Link-AMG solver Package (Mehl and Hill, 2001)
Output Control Option
Ground-Water Transport Process
Sensitivity Process
Observation Process
Parameter-Estimation Process

SUMMARY

Computer models of ground-water flow require input data to define the simulated flow system. This report describes a data-input program, MFI2K, developed by the U.S. Geological Survey (USGS) for the USGS modular three-dimensional finite-difference ground-water model, MODFLOW-2000. MFI2K is designed to be easy to use and to run on personal computers. Data are entered interactively through a series of display screens.

MFI2K supports the solute-transport and parameter-estimation capabilities of MODFLOW-2000. MFI2K also supports the MODPATH particle-tracking program. Other data-entry programs can be used in conjunctions with MFI2K. User instructions are provided in this report. MFI2K can be obtained from the USGS (see report preface).

REFERENCES CITED

Goode, D.J., and Appel, C.A., 1992, Finite-difference interblock transmissivity for unconfined aquifers and for aquifers having smoothly varying transmissivity: U.S. Geological Survey Water-Resources Investigations Report 92-4124, 79 p.

Harbaugh, A.W., 1994, A data input program (MFI) for the U.S. Geological Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 94-468, 24 p.

_____1995, Direct solution package based on alternating diagonal ordering for the U.S. Geological Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 95-288, 46 p.

Harbaugh, A.W., Banta, E.R., Hill, M.C., and McDonald, M.G., 2000, MODFLOW-2000, the U.S. Geological Survey modular ground-water model—User guide to modularization concepts and the ground-water flow process: U.S. Geological Survey Open-File Report 00-92, 121 p.

Hill, M.C., 1990, Preconditioned conjugate-gradient 2 (PCG2), a computer program for solving ground-water flow equations: U.S. Geological Survey Water-Resources Investigations Report 90-4048, 43 p.

_____1998, Methods and guidelines for effective model calibration: U.S. Geological Survey Water-Resources Investigations Report 98-4005, 90 p.

Hill, M.C., Banta, E.R., Harbaugh, A.W., and Anderman, E.R., 2000, MODFLOW-2000, the U.S. Geological Survey modular ground-water model—User guide to the observation, sensitivity, and parameter-estimation processes and three post-processing programs: U.S. Geological Survey Open-File Report 00-184, 209 p.

Interactive Software Services, 2000, Winteracter Subroutine Reference: Interactive Software Services Ltd.

Konikow, L.F., Goode, D.J., and Hornberger, G.Z., 1996, A three-dimensional method-of-characteristics solute-transport model (MOC3D): U.S. Geological Survey Water-Resources Investigations Report 96-4267, 87 p.

Mehl, S.W., and Hill, M.C., 2001, MODFLOW-2000, the U.S. Geological Survey modular ground-water model—user guide to the Link-AMG (LMG) Package for solving matrix equations using an algebraic multigrid solver: U.S. Geological Survey Open-File Report 01-177, 33 p.

Pollock, D.W., 1994, User's guide for MODPATH/MODPATH-PLOT, Version 3: A particle tracking post-processing package for MODFLOW, the U.S. Geological Survey finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 94-464, 6 ch.

Appendix – MFI2K Help Information

This appendix contains help information for each screen. The information is organized like the MFI2K Main Menu. This appendix will be distributed as a separate file with the MFI2K software so that the help information can be examined interactively while MFI2K is running. References cited in this appendix are listed in the References Cited section. Although this help information is more complete than the help provided on the MFI2K screens, additional information still may be required. The user should consult the appropriate MODFLOW-2000 or MODPATH documentation for additional information.

FILE

Save As
The dataset is saved using a new name, and MFI2K continues editing the new dataset. The old dataset is left as is.

Save
The dataset is saved using the current name. The old dataset is overwritten.

Run MF2K
Execute MODFLOW-2000 using the current dataset. The current dataset is saved first.

Abort
MFI2K is exited without saving the data. Any changes made to the data since a "Save As", "Save" or "Run MF2K" menu item was used will be lost. The user will be prompted to determine if he really wants to do this.

Exit (and Save)
The dataset is saved and MFI2K is exited. If some data are incomplete, the user is prompted and allowed to go back into the main menu. If the user goes ahead and exits with incomplete data, MFI2K will pick up again where the user left off the next time the dataset is edited.

OPTIONS

Check Complete
All of the active MODFLOW simulation options are displayed and a status flag is shown for each option that indicates whether or not data entry is complete. For any option that is incomplete, the specific missing data can be displayed by using the Check pushbutton on the data-editing screen where the data for that MODFLOW option is entered.

Deactivate
This option deactivates (turns off) MODFLOW options. Using a data-editing screen automatically turns on the corresponding option. For example, selecting RCH in the STRESS menu turns on RCH (recharge). The Deactivate option allows recharge to be turned off.

Show Files
The names of all files that are being used for the MODFLOW simulation are displayed.

GLOBAL/LIST Files
This option allows the names of the GLOBAL and LIST files to be specified.

Zone-Mult/ Multiplier Arrays

The multiplier file defines two-dimensional arrays that are used to define array parameters. MFI2K does not allow multiplier-array functions to be edited; however, if an existing dataset includes functions, these are maintained when MFI2K saves the dataset.

The "Select Multiplier Array" list allows a multiplier array to be selected for editing. The following editing options allow the values of each array element to be defined:

- Constant—all elements of the array have the same value.
- Package—data are saved in the multiplier file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

The "ADD" pushbutton allows a new multiplier array to be created.

The "Delete" pushbutton causes the currently selected multiplier array to be deleted.

The "Comments" pushbutton allows comments to be defined. These comments are placed at the beginning of the multiplier file.

Zone-Mult/ Zone Arrays

The zone file defines two-dimensional arrays that are used to define array parameters

The "Select Zone Array" list allows a zone array to be selected for editing. The following options allow the values of the array to be defined:

- Constant—all elements of the array have the same value.
- Package—data are saved in the zone file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

The "ADD" pushbutton allows a new zone array to be created.

The "Delete" pushbutton causes the currently selected zone array to be deleted.

The "Comments" pushbutton allows comments to be defined. These comments are placed at the beginning of the zone file.

DIS

Discretization File. For the input variables that are arrays, the following editing options allow the values of each array element to be defined:

- Constant—all elements of the array have the same value.
- Package—data are saved in the DIS file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Time and Length Units

The time unit of model data must be consistent for all data values that involve time. For example, if years is the chosen time unit, stress-period length, time-step length, transmissivity, and so on, all must be expressed using years for their time units. Note that the program still will run even if "undefined" time units are specified because the fundamental equations used in MODFLOW do not require that the time

unit be identified. But be sure to use consistent units for all input data even when ITMUNI indicates an undefined time unit. When the time unit is defined, MODFLOW uses the time unit to print a table of elapsed simulation time. The acceptable values are:

Undefined	Hours
Seconds	Days
Minutes	Years

The length unit of model data must be consistent for all data values that involve length. For example, if feet is the chosen length unit, grid spacing, head, hydraulic conductivity, water volumes, and so forth, all must be expressed using feet for their length units. Note that the program still will run even if "undefined" length units are specified because the fundamental equations used in MODFLOW do not require that the length unit be identified. But be sure to use consistent units for all input data even when LENUNI indicates an undefined length unit. The acceptable values are:

Undefined
Feet
Meters
Centimeters

DELR
DELR is the cell width along rows. Read one value for each of the NCOL columns. This is a one-dimensional variable with one value for each column.

DELC
DELC is the cell width along columns. Read one value for each of the NROW rows. This is a one-dimensional variable with one value for each row.

LAYCBD
LAYCBD indicates whether or not a layer has a Quasi-3D confining bed below it. "No" indicates no confining bed, and "Yes" indicates a confining bed. LAYCBD for the bottom layer must be "No."

TOP
Top is the top elevation of layer 1. This is a two-dimensional array. For the common situation in which the top layer represents a water-table aquifer, setting Top equal to land-surface elevation may be reasonable.

BOTM
BOTM is the bottom elevation of a model layer or a Quasi-3D confining bed. This is a set of two-dimensional arrays.

Stress Periods
"Number of Stress Periods" is the number of stress periods in the simulation (variable NPER).

"Length" is the length of a stress period (variable PERLEN).

"Steps" is the number of time steps in a stress period (variable NSTP).

"Multiplier" is the multiplier for the length of successive time steps (variable TSMULT). The length of a time step is calculated by multiplying the length of the previous time step by TSMULT. The length of the first time step, Δt_1, is related to PERLEN, NSTP, and TSMULT by the relation:

$$\Delta t_1 = \text{PERLEN}\ (\text{TSMULT}-1)/(\text{TSMULT}^{\text{NSTP}}-1)$$

Ss/tr is a character variable that indicates whether the stress period is transient or steady state. The only allowed options are “SS” and “TR”, but these are case insensitive.

Comments

Comments are placed at the beginning of the DIS file.

BAS

Basic Package.

Check Data

This option checks the BAS Package data to determine whether data are complete. If not complete, the incomplete data are listed.

Miscellaneous

The “Comments” field allows comments, which are placed at the beginning of the BAS Package file, to be defined. The first two comment lines will become variable HEADNG, which is used as a printout title throughout the program. (If there are no comment lines, then HEADNG will be blank.) HEADNG is limited to 80 columns, but subsequent Text lines can be up to 199 columns. Any character can be included in Text. The “#” character must be in column 1.

HNOFLO is the value of head to be assigned to all inactive (no flow) cells (IBOUND = 0) throughout the simulation. Because head at inactive cells is unused in model calculations, this does not affect model results but serves to identify inactive cells when head is printed. This value also is used as drawdown at inactive cells if the drawdown option is used. Even if the user does not anticipate having inactive cells, a value for HNOFLO must be entered.

Format flag indicates whether fixed or free format is used for input variables throughout the Basic Package and other packages as indicated in their input instructions.

IBOUND

IBOUND is the boundary variable. One value is read for every model cell. Usually, these values are read a layer at a time; however, when the XSECTION option is specified, a single array for the cross section is read. Note that although IBOUND is read as one or more two-dimensional variables, it is stored internally as a three-dimensional variable.

If IBOUND(J,I,K) < 0, cell J,I,K has a constant head.
If IBOUND(J,I,K) = 0, cell J,I,K is inactive (no flow).
If IBOUND(J,I,K) > 0, cell J,I,K is active (variable head).

The following editing options allow the IBOUND values to be defined for each layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the BAS file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Initial Head

Initial head is the head at the beginning of the simulation, which is variable STRT. STRT must be specified for all simulations, including steady-state simulations. One value is read for every model cell. Usually, these values are read one layer at a time. When the XSECTION option is specified, however, a single array for the cross section is read. For simulations in which the first stress period is steady state, the values used for STRT generally do not affect the simulation [exceptions may occur if cells go dry and (or)

rewet]. The execution time, however, will be less if STRT includes hydraulic heads that are close to the steady-state solution.

The following editing options allow the STRT values to be defined for each layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the BAS file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Internal Flow/ BCF

Block-Centered Flow Package

Check Data

This option causes MFI2K to check the BCF Package data to determine if data are complete. If not, the incomplete data are listed.

Miscellaneous

Head at cells that go dry (variable HDRY) is the head that is assigned to cells that are converted to dry during a simulation. Although this value is not used in the model calculations, HDRY is useful as an indicator when looking at the resulting heads that are output from the model. HDRY is, thus, similar to HNOFLO in the Basic Package, which is the value assigned to cells that are no-flow cells at the start of a model simulation.

OFF and ON Wetting Capability options—OFF indicates that wetting is turned off, and ON indicates that wetting is turned on.

WETFCT is a factor that is included in the calculation of the head that initially is established at a cell when the cell is converted from dry to wet. (See IHDWET.)

IWETIT is the iteration interval for attempting to wet cells. Wetting is attempted every IWETIT iteration. If using the PCG solver (Hill, 1990), this value applies to outer iterations, not inner iterations. If IWETIT is 0, the value is changed to 1.

IHDWET is an option that determines which equation is used to define the initial head at cells that become wet:

$BOT + WETFCT (h_n - BOT)$
$BOT + WETFCT (WETDRY)$

LAYCON

The LAYCON option activates a screen that is used to specify three values for each layer of the model grid:

LAYCON is the layer type:

- Confined—Transmissivity and storage coefficient of the layer are constant for the entire simulation (LAYCON = 0).
- Unconfined—Transmissivity of the layer varies (LAYCON = 1) and is calculated from the saturated thickness and hydraulic conductivity. The storage coefficient is constant. This type code is valid only for layer 1.
- Partially Convertible—Transmissivity of the layer is constant, but the storage coefficient may alternate between confined and unconfined values (LAYCON = 2). Vertical flow from above is limited if the layer desaturates.

- Fully Convertible—Transmissivity of the layer varies, and the storage coefficient may alternate between confined and unconfined values (LAYCON = 3). Transmissivity is calculated from the saturated thickness and hydraulic conductivity. Vertical flow from above is limited if the layer desaturates.

Horizontal Anisotropy (Variable TRPY) is the ratio of transmissivity or hydraulic conductivity (whichever is being used for input) in the Y direction (along a column) to transmissivity or hydraulic conductivity in the X direction (along a row). Specify 1.0 for isotropic layers.

LAYAVG defines the method of calculating interblock transmissivity. The methods are described by Goode and Appel (1992).

- Harmonic (LAYAVG = 0)—Harmonic mean
- Arithmetic (LAYAVG = 1)—Arithmetic mean
- Logarithmic (LAYAVG = 2)—Logarithmic mean
- Arith-log (LAYAVG = 3) —Arithmetic mean of saturated thickness and logarithmic-mean hydraulic conductivity.

Hydraulic Data

This screen allows hydraulic arrays to be entered for each layer as required according to the options in effect such as steady state versus transient, wetting on or off, and layer type. The following editing options allow the array values to be defined for each layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the BCF file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Sf1 is the primary storage coefficient. Read only if there are one or more transient stress periods specified in the Discretization File. For LAYCON equal to 1, Sf1 always will be specific yield, whereas for LAYCON equal to 2 or 3, Sf1 always will be confined storage coefficient. For LAYCON equal to 0, Sf1 would normally be confined storage coefficient; however, a LAYCON value of 0 also can be used to simulate unconfined conditions where drawdowns are expected to remain everywhere a small fraction of the saturated thickness, and where there is no layer above, or flow from above is negligible. In this case, specific yield values would be entered for Sf1.

Tran is the transmissivity along rows. Tran is multiplied by TRPY to obtain transmissivity along columns. Read only for layers where LAYCON is 0 or 2.

HY is the hydraulic conductivity along rows. HY is multiplied by TRPY to obtain hydraulic conductivity along columns. Read only for layers where LAYCON is 1 or 3.

Vcont is the vertical hydraulic conductivity divided by the thickness of a layer to the layer below. The value for a cell is the hydraulic conductivity divided by thickness for the material between the node in that cell and the node in the cell below. Because there is no layer beneath the bottom layer, Vcont cannot be specified for the bottom layer.

Sf2 is the secondary storage coefficient. Read only for layers where LAYCON is 2 or 3 and only if there are one or more transient stress periods specified in the Discretization File. The secondary storage coefficient always is specific yield.

WETDRY is a combination of the wetting threshold and a flag to indicate which neighboring cells can cause a cell to become wet. If WETDRY < 0, only the cell below a dry cell can cause the cell to become wet. If WETDRY > 0, the cell below a dry cell and the four horizontally adjacent cells can cause a cell to

become wet. If WETDRY is 0, the cell cannot be wetted. The absolute value of WETDRY is the wetting threshold. When the sum of BOT and the absolute value of WETDRY at a dry cell is equaled or exceeded by the head at an adjacent cell, the cell is wetted. Read only if LAYCON is 1 or 3 and IWDFLG is not 0.

Internal Flow/ LPF

The Layer-Property Flow Package (LPF) is an alternative to the BCF Package. These packages should not be used simultaneously.

Check

This option causes MFI2K to check the LPF Package data to determine if data are complete. If not complete, the incomplete data are listed.

Miscellaneous

Head assigned to cells that convert to dry (variable HDRY) is the head that is printed or saved at cells that have converted to dry during a simulation. Although this value is not used in the model calculations, it is useful as an indicator when looking at the resulting heads that are output from the model. HDRY is, thus, similar to HNOFLO in the Basic Package, which is the value assigned to cells that are no-flow cells at the start of a model simulation.

Factor that affects initial head when cells become wet (WETFCT) is a variable that is included in the equation for the head that initially is established at a cell when it is converted from dry to wet. (See IHDWET.)

Iteration interval for attempting to wet cells (IWETIT) determines the iterations at which wetting is attempted at wettable cells. Wetting is attempted every IWETIT iteration. If using the PCG solver (Hill, 1990), this value applies to outer iterations, not inner iterations. If IWETIT is 0, it is changed to 1.

Equation to define initial head when cells become wet (IHDWET) is an option that determines which equation defines the initial head at cells that convert from dry to wet:

BOT + WETFCT (h_n - BOT)
BOT + WETFCT (WETDRY)

LAYTYP

The LAYTYP option activates a screen that is used to specify four values for each layer of the model grid:

LAYTYP is the layer type:

- Confined—Transmissivity and storage coefficient of the layer are constant for the entire simulation (LAYTYP = 0).
- Convertible—Transmissivity of the layer varies, and the storage coefficient may alternate between confined and unconfined values (LAYTYP ≠ 0). Transmissivity is calculated from the saturated thickness and hydraulic conductivity. Vertical flow from above is limited if the layer desaturates. For the water table, specify convertible and be sure that the top elevation is higher than the computed head.

LAYAVG defines the method of calculating interblock transmissivity. The methods are described by Goode and Appel (1992).

- Harmonic (LAYAVG = 0)—Harmonic mean (the method used in MODFLOW-88).
- Logarithmic (LAYAVG = 1) —Logarithmic mean
- Arith-log (LAYAVG = 2) —Arithmetic mean of saturated thickness and logarithmic-mean hydraulic conductivity.

CHANI (horizontal anisotropy) is the ratio of hydraulic conductivity in the Y direction (along a column) to hydraulic conductivity in the X direction (along a row). A nonzero value here applies to all cells in the layer. Specify 1.0 for isotropic layers. Specify 0.0 in order to use array HANI to specify individual values for every cell in the layer through the Hydraulic Data screen.

LAYVKA is a flag indicating whether array VKA is vertical hydraulic conductivity or the ratio of horizontal to vertical hydraulic conductivity.

LAYWET is the wetting flag. Wetting can be on or off for each layer. Wetting cannot be on for a confined layer.

Hydraulic Data

This screen allows hydraulic arrays to be entered for each layer as required according to the options in effect such as steady state versus transient, wetting on or off, and layer type. Some of these arrays can be defined using the following parameters:

- HK is the parameter type for defining array HK
- VK is the parameter type for defining VKA when VKA is vertical hydraulic conductivity
- VANI is the parameter type for defining VKA when VKA is the ratio of horizontal to vertical hydraulic conductivity
- SS is the parameter type for defining array Ss
- SY is the parameter type for defining array Sy
- VKCB is the parameter type for defining array VKCB
- HANI is the parameter type for defining array HANI

If parameters are not used to define an array, then the values are defined as two-dimensional arrays for each layer in which the array is required. The following editing options allow the array values to be defined for each layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the LPF file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

If an array is defined using parameters, then all values of the array must be defined using parameters. The parameters are defined by specifying a parameter name, parameter type, parameter value, and one or more clusters that specify the layer, multiplier array, zone array, and zone codes that are associated with the parameter.

HY is the hydraulic conductivity along rows. HY is multiplied by HANI or CHANI to obtain hydraulic conductivity along columns.

HANI is the ratio of hydraulic conductivity along columns (Y direction) to the hydraulic conductivity along rows (X direction). This array is only specified for layers in which CHANI is 0.0.

VKCB is the vertical hydraulic conductivity of a Quasi 3-D confining bed. This array is only defined for layers that are underlain by a Quasi-3D confining bed.

VKA is the vertical hydraulic conductivity or the ratio of horizontal hydraulic conductivity (HY) to vertical hydraulic conductivity. The type of data depends on the value of LAYVKA for each layer.

Ss is the specific storage. This array is only required when there is at least one transient stress period.

Sy is the specific yield. This array is only required when there is at least one transient stress period and for layers that are convertible.

WETDRY is a combination of the wetting threshold and a flag to indicate which neighboring cells can cause a cell to become wet. If WETDRY < 0, only the cell below a dry cell can cause the cell to become wet. If WETDRY > 0, the cell below a dry cell and the four horizontally adjacent cells can cause a cell to become wet. If WETDRY is 0, the cell cannot be wetted. The absolute value of WETDRY is the wetting threshold. When the sum of BOT and the absolute value of WETDRY at a dry cell is equaled or exceeded by the head at an adjacent cell, the cell is wetted. This array is required only for layers that are wettable.

Print Codes

This option allows print codes for each layer to be specified for use with parameters. The print codes specify the format for printing the resulting input values after the values are created from parameters. If any array is not determined from parameters, then these print codes have no effect on print format. The codes are:

0 - 10G11.4	11 - 20F5.4
1 - 11G10.3	12 - 10G11.4
2 - 9G13.6	13 - 10F6.0
3 - 15F7.1	14 - 10F6.1
4 - 15F7.2	15 - 10F6.2
5 - 15F7.3	16 - 10F6.3
6 - 15F7.4	17 - 10F6.4
7 - 20F5.0	18 - 10F6.5
8 - 20F5.1	19 - 5G12.5
9 - 20F5.2	20 - 6G11.4
10 - 20F5.3	21 - 7G9.2

Comments

Comments are placed at the beginning of the LPF file.

STRESS/ Check

Check all stress data for missing data.

River Package

When the external editing mechanism is used to define river reaches with or without parameters, the following fields must be defined for each river reach:

Layer—the layer number of the cell containing the river reach.
Row—the row number of the cell containing the river reach.
Column—the column number of the cell containing the river reach.
Stage—the head in the river.
Condfact or Cond—When parameters are used, Condfact is the factor used to calculate riverbed hydraulic conductance from the parameter value. The conductance is the product of Condfact and the parameter value. When parameters are not used, Cond is the riverbed conductance.
Rbot—the elevation of the bottom of the riverbed.
IFACE—a flag for use with MODPATH that defines the cell face through which an external source/sink flows. This field is automatically added if MODPATH is activated. IFACE values are:

0—flow is distributed internally.
1—flow is applied to the left face.
2—flow is applied to the right face.
3—flow is applied to the front face.
4—flow is applied to the back face.
5—flow is applied to the bottom face.
6—flow is applied to the top face.

The "Select Stress Period" list shows all stress periods in the simulation and allows a specific period to be selected.

Parameter Data

On the "Parameter data" half of the screen, a list shows all the river parameters that have been defined and allows a specific parameter to be selected. The list also shows whether a parameter is active (being used) in the selected stress period.

Five pushbuttons are used to define parameters and control the stress periods in which they are used:

- "Deactivate this stress period"—deactivates the selected parameter in the selected stress period.
- "Activate this stress period"—makes the selected parameter active in the selected stress period.
- "Modify"—allows the selected parameter to be modified.
- "New"—allows a new parameter to be defined.
- "Delete"—deletes the selected parameter.

There are two options for specifying the river data for a parameter:

- Separate—allows river data to be located in a file that MFI2K does not read, and MFI2K cannot modify that file. Rather, MFI2K sets up the dataset so that MODFLOW will read the file.
- Package—nonparameter river data are saved in the RIV Package file, and the external editing mechanism is used to modify the data.

When a parameter is first defined using the New pushbutton, the parameter is defined as using the Package option with 0 reaches.

Nonparameter Data

Nonparameter river reaches can be defined in addition to the reaches defined by parameters. The choices for defining nonparameter reaches are:

- None—no nonparameter river reaches are being used in the selected stress period.
- Previous—nonparameter river reaches from the previous stress period are reused.
- Package—nonparameter river data are saved in the RIV Package file, and the external editing mechanism is used to modify the data. The fields that must be defined for each reach are the same as for parameters except that Condfact is replaced with the actual riverbed conductance.
- Separate—nonparameter river data are stored in a separate file that MFI2K does not read.

The Comments pushbutton allows comments to be edited, which are placed at the beginning of the RIV file.

STRESS/ WEL

Well Package

When the external editing mechanism is used with or without parameters, the following fields must be defined for each well:

Layer—the layer number of the cell containing the well.
Row—the row number of the cell containing the well.
Column—the column number of the cell containing the well.
Qfact or Q—When parameters are used, Qfact is the factor used to calculate well recharge rate (negative value indicates pumping) from the parameter value. The recharge rate is the product of Qfact and the parameter value. When parameters are not used, Q is the well recharge rate (negative value indicates pumping)
IFACE—a flag for use with MODPATH that defines the cell face through which an external source/sink flows. This field automatically is added if MODPATH is activated. IFACE values are:

0—flow is distributed internally.
1—flow is applied to the left face.
2—flow is applied to the right face.
3—flow is applied to the front face.
4—flow is applied to the back face.
5—flow is applied to the bottom face.
6—flow is applied to the top face.

The "Select Stress Period" list shows all stress periods in the simulation and allows a specific period to be selected.

Parameter Data

On the "Parameter data" half of the screen, a list shows all the well parameters that have been defined and allows a specific parameter to be selected. The list also shows whether a parameter is active (being used) in the selected stress period.

Five pushbuttons are used to define parameters and control the stress periods in which they are used:

- "Activate this stress period"—makes the selected parameter active in the selected stress period.
- "Modify"—allows the selected parameter to be modified.
- "New"—allows a new parameter to be defined.
- "Delete"—deletes the selected parameter.
- "Deactivate this stress period"—deactivates the selected parameter in the selected stress period.

Two options are available for specifying the well data for a parameter:

- Separate—allows well data to be located in a file that MFI2K does not read, and MFI2K cannot modify that file. Rather, MFI2K sets up the dataset so that MODFLOW will read the file.
- Package—well data are saved in the WEL Package file, and the external editing mechanism is used to modify the data.

A parameter, first defined using the New pushbutton, is defined as using the Package option with 0 wells.

Nonparameter Data

Nonparameter wells can be defined in addition to the wells defined by parameters. The choices for defining nonparameter wells are:

- None—no nonparameter wells are being used in the selected stress period.
- Previous—nonparameter wells from the previous stress period are reused.
- Package—nonparameter well data are saved in the WEL Package file, and the external editing mechanism is used to modify the data. The fields that must be defined for each well are the same as for parameters except that Qfact is replaced with the actual well recharge (negative value indicates discharge).
- Separate—nonparameter well data are stored in a separate file that MFI2K does not read.

The Comments pushbutton allows comments, which are placed at the beginning of the WEL file, to be edited.

STRESS/ RCH

Recharge Package

The "Depth Option" list allows the vertical location for applying recharge to be specified:

- Top Layer—recharge is applied to layer 1.
- Specified Layers—recharge is applied to the layer specified in two-dimensional array IRCH. When this option is selected, IRCH appears in the "Array Name" list.
- Automatic Selection—recharge passes vertically through no-flow cells until it reaches a variable-head cell or a constant-head cell. A constant-head cell intercepts the recharge and prevents deeper infiltration.

The "Select Stress Period" list shows all stress periods in the simulation and allows a specific period to be selected.

The "Select Array" list shows the two-dimensional arrays that must be defined without parameters and allows an array to be selected. The RECH array can be defined with or without parameters (but not both). If parameters are defined in the RCH Package, they apply to RECH. Thus, RECH does not appear in the Array Name list if there are any RCH parameters defined.

Parameter Data

On the "Parameter data" half of the screen, a list shows all the recharge parameters that have been defined and allows a specific parameter to be selected. The list also shows whether a parameter is active (being used) in the selected stress period.

Five pushbuttons are used to define parameters and control the stress periods in which they are used:

- "Activate parameter this stress period"—makes the selected parameter active in the selected stress period.
- "Modify"—allows the selected parameter to be modified.
- "New"—allows a new parameter to be defined.

- "Delete"—deletes the selected parameter.
- "Deactivate Parameter this stress period"—deactivates the selected parameter in the selected stress period.

Nonparameter Data

Nonparameter arrays are defined the same way as other two-dimensional arrays in MFI2K. The choices for defining nonparameter arrays are:

- Previous—nonparameter data from the previous stress period are reused.
- Constant—all cells have the same value.
- Package—nonparameter data are saved in the RCH Package file, and the external editing mechanism is used to modify the data.
- Separate—nonparameter data are stored in a separate file that MFI2K does not read.

The Comments pushbutton allows comments, which are placed at the beginning of the RCH file, to be edited.

STRESS/ DRN

Drain Package

When the external editing mechanism is used with or without parameters, the following fields must be defined for each drain:

Layer—the layer number of the cell containing the drain.
Row—the row number of the cell containing the drain.
Column—the column number of the cell containing the drain.
Elevation—the elevation of the drain.
Condfact or Cond—When parameters are used, Condfact is the factor used to calculate drain conductance from the parameter value. The drain conductance is the product of Condfact and the parameter value. When parameters are not used, Cond is the drain conductance.
IFACE—a flag for use with MODPATH that defines the cell face through which an external source/sink flows. This field automatically is added if MODPATH is activated. IFACE values are:

0—flow is distributed internally.
1—flow is applied to the left face.
2—flow is applied to the right face.
3—flow is applied to the front face.
4—flow is applied to the back face.
5—flow is applied to the bottom face.
6—flow is applied to the top face.

The "Select Stress Period" list shows all stress periods in the simulation and allows a specific period to be selected.

Parameter Data

On the "Parameter data" half of the screen, a list shows all the drain parameters that have been defined and allows a specific parameter to be selected. The list also shows whether a parameter is active (being used) in the selected stress period.

Several pushbuttons are used to define parameters and control the stress periods in which they are used:

- "Activate this stress period"—makes the selected parameter active in the selected stress period.
- "Modify"—allows the selected parameter to be modified.
- "New"—allows a new parameter to be defined.
- "Delete"—deletes the selected parameter.
- "Deactivate this stress period"—deactivates the selected parameter in the selected stress period.

Two options are available for specifying the drain data for a parameter:

- Separate—allows drain data to be located in a file that MFI2K does not read, and MFI2K cannot modify that file. Rather, MFI2K sets up the dataset so that MODFLOW will read the file.
- Package—drain data are saved in the DRN Package file, and the external editing mechanism is used to modify the data.

A parameter, first defined using the New pushbutton, is defined as using the Package option with 0 drains.

Nonparameter Data

Nonparameter drains can be defined in addition to the drains defined by parameters. The choices for defining nonparameter drains are:

- None—no nonparameter drains are being used in the selected stress period.
- Previous—nonparameter drains from the previous stress period are reused.
- Package—nonparameter drain data are saved in the DRN Package file, and the external editing mechanism is used to modify the data. The fields that must be defined for each drain are the same as for parameters except that Condfact is replaced with the actual drain conductance.
- Separate—nonparameter drain data are stored in a separate file that MFI2K does not read.

The Comments pushbutton allows comments, which are placed at the beginning of the DRN file, to be edited.

STRESS/ GHB

General-Head Boundary Package

When the external editing mechanism is used, the following fields must be defined for each boundary:

Layer—the layer number of the cell containing the boundary.
Row—the row number of the cell containing the boundary.
Column—the column number of the cell containing the boundary.
Bhead—the head on the boundary.
Condfact or Cond—When parameters are used, Condfact is the factor used to calculate boundary conductance from the parameter value. The boundary conductance is the product of Condfact and the parameter value. When parameters are not used, Cond is the boundary conductance.
IFACE—a flag for use with MODPATH that defines the cell face through which an external source/sink flows. This field is automatically added if MODPATH is activated. IFACE values are:

0—flow is distributed internally.
1—flow is applied to the left face.
2—flow is applied to the right face.
3—flow is applied to the front face.
4—flow is applied to the back face.
5—flow is applied to the bottom face.
6—flow is applied to the top face.

The "Select Stress Period" list shows all stress periods in the simulation and allows a specific period to be selected.

Parameter Data

On the "Parameter data" half of the screen, a list shows all the GHB parameters that have been defined and allows a specific parameter to be selected. The list also shows if a parameter is active (being used) in the selected stress period.

Several pushbuttons are used to define parameters and control the stress periods in which they are used:

- "Activate this stress period"—makes the selected parameter active in the selected stress period.
- "Modify"—allows the selected parameter to be modified.
- "New"—allows a new parameter to be defined.
- "Delete"—deletes the selected parameter.
- "Deactivate this stress period"—deactivates the selected parameter in the selected stress period.

Two options are available for specifying the boundary data for a parameter:

- Separate—allows boundary data to be located in a file that MFI2K does not read, and MFI2K cannot modify that file. Rather, MFI2K sets up the dataset so that MODFLOW will read the file.
- Package—boundary data are saved in the GHB Package file, and the external editing mechanism is used to modify the data.

A parameter, first defined using the New pushbutton, is defined as using the Package option with 0 boundaries.

Nonparameter Data

Nonparameter boundaries can be defined in addition to the boundaries defined by parameters. The choices for defining nonparameter boundaries are:

- None—no nonparameter boundaries are being used in the selected stress period.
- Previous—nonparameter boundaries from the previous stress period are reused.
- Package—nonparameter boundary data are saved in the GHB Package file, and the external editing mechanism is used to modify the data. The fields that must be defined for each boundary are the same as for parameters except that Condfact is replaced with the actual boundary conductance.
- Separate—nonparameter boundary data are stored in a separate file that MFI2K does not read.

The Comments pushbutton allows comments, which are placed at the beginning of the GHB file, to be edited.

STRESS/ EVT

Evapotranspiration Package

The "Depth Option" list allows the vertical location for applying evapotranspiration to be specified:

- Top Layer—evapotranspiration is applied to layer 1.
- Specified Layers—evapotranspiration is applied to the layer specified in two-dimensional array IEVT. When this option is selected, IEVT appears in the "Array Name" list.

The "Select Stress Period" list shows all stress periods in the simulation and allows a specific period to be selected.

The "Select Array" list shows the two-dimensional arrays that must be defined without parameters and allows an array to be selected. The EVTR array can be defined with or without parameters (but not both). If parameters are defined in the EVT Package, they apply to EVTR. Thus, EVTR does not show up in the

Array Name list if any EVT parameters are defined. The other arrays to be defined are SURF, EXDP, and optionally IEVT.

Parameter Data

On the "Parameter data" half of the screen, a list shows all the evapotranspiration parameters that have been defined and allows a specific parameter to be selected. The list also shows whether a parameter is active (being used) in the selected stress period.

Nonparameter Data

Five pushbuttons are used to define parameters and control the stress periods in which they are used:

- "Activate parameter this stress period"—makes the selected parameter active in the selected stress period.
- "Modify"—allows the selected parameter to be modified.
- "New"—allows a new parameter to be defined.
- "Delete"—deletes the selected parameter.
- "Deactivate Parameter this stress period"—deactivates the selected parameter in the selected stress period.

Nonparameter arrays are defined the same way as other two-dimensional arrays in MFI2K. The choices for defining nonparameter arrays are:

- Previous—nonparameter data from the previous stress period are reused
- Constant—all cells have the same value.
- Package—nonparameter data are saved in the EVT Package file, and the external editing mechanism is used to modify the data.
- Separate—nonparameter data are stored in a separate file that MFI2K does not read.

The Comments pushbutton allows comments, which are placed at the beginning of the EVT file, to be edited.

SOLVER

The solver screen allows one of five solvers to be selected for solving the ground-water and sensitivity simultaneous equations:

PCG

MXITER is the maximum number of outer iterations—that is, calls to the solution routine. For a linear problem MXITER should be 1, unless more than 50 inner iterations are required, when MXITER could be as large as 10. A larger number (generally less than 100) is required for a nonlinear problem.

ITER1 is the number of inner iterations. For nonlinear problems, ITER1 usually ranges from 10 to 30; a value of 30 will be sufficient for most linear problems.

IPRPCG is the printout interval for PCG. If IPRPCG is equal to 0, the variable is changed to 999. The maximum head change (positive or negative) and residual change are printed for each iteration of a time step whenever the time step is an even multiple of IPRPCG. This printout also occurs at the end of each stress period regardless of the value of IPRPCG.

MUTPCG is a flag that controls printing of convergence information from the solver:

0—is for printing tables of maximum head change and residual every iteration.
1—is for printing only the total number of iterations.
2—is for no printing.

3—is for printing only if convergence fails.

HCLOSE is the head change criterion for convergence, in units of length. When the maximum absolute value of head change from all nodes during an iteration is less than or equal to HCLOSE, and the criterion for RCLOSE also is satisfied (see below), iteration stops.

RCLOSE is the residual criterion for convergence, in units of cubic length per time. When the maximum absolute value of the residual at all nodes during an iteration is less than or equal to RCLOSE, and the criterion for HCLOSE also is satisfied (see above), iteration stops.

For nonlinear problems, convergence is achieved when the convergence criteria are satisfied for the first inner iteration.

RELAX is the relaxation parameter used with NPCOND = 1. Usually, RELAX = 1.0, but for some problems a value of 0.99, 0.98, or 0.97 will reduce the number of iterations required for convergence. RELAX is not used if NPCOND is not 1.

DAMP is the damping factor. The damping factor typically is set equal to 1.0, which indicates no damping. A value less than 1.0 and greater than 0.0 causes damping.

SIP

MXITER is the maximum number of times through the iteration loop in one time step in an attempt to solve the system of finite-difference equations.

HCLOSE is the head change criterion for convergence. When the maximum absolute value of head change from all nodes during an iteration is less than or equal to HCLOSE, iteration stops.

ACCL is the acceleration variable. The acceleration variable must be greater than 0.0 and is generally equal to 1.0. If 0.0 is entered, it is changed to 1.0.

WSEED is the seed for calculating iteration variables. If a value of 0.0 is entered, MFI2K will specify input data such that SIP will calculate the seed.

IPRSIP—is the printout interval for SIP. If IPRSIP is equal to 0, the variable is changed to 999. The maximum head change (positive or negative) is printed for each iteration of a time step whenever the time step is an even multiple of IPRSIP. This printout also occurs at the end of each stress period regardless of the value of IPRSIP.

SOR

MXITER is the maximum number of iterations allowed in a time step.

HCLOSE is the head change criterion for convergence. When the maximum absolute value of head change from all nodes during an iteration is less than or equal to HCLOSE, iteration stops.

ACCL is the acceleration variable, usually between 1.0 and 2.0.

IPRSOR is the printout interval for SOR. IF IPRSOR is equal to 0, the interval is changed to 999. The maximum head change (positive or negative) is printed for each iteration of a time step whenever the time step is an even multiple of IPRSOR. This printout also occurs at the end of each stress period regardless of the value of IPRSOR.

ITMX—is the maximum number of iterations for each time step. Specify ITMX = 1 if iteration is not desired. Ideally, iteration would not be required for direct solution; however, the iteration is necessary if the flow equation is nonlinear (see explanation for IFREQ = 3) or if computer precision limitations result in inaccurate calculations as indicated by a large water budget error (>1% for a 10,000-cell grid). For a nonlinear flow equation, each iteration is equally time consuming because [A] is changed at the start of each iteration and Gaussian elimination is required after each change. Performing Gaussian elimination every iteration is called external iteration. For a linear equation, iteration is appreciably faster because [A] is changed, at most, once per time step; thus, Gaussian elimination is required, at most, once per time step. Iteration without performing Gaussian elimination every iteration is called internal iteration.

IFREQ is a flag indicating the frequency at which coefficients in [A] change. This affects the efficiency of solution; appreciable work can be avoided if [A] is known to remain constant all or part of the time.

IFREQ = 1 indicates that the flow equations are linear and that coefficients of simulated head for all stress terms are constant for all stress periods. To meet the linearity requirement, all model layers must be confined (which is specified in the Block-Centered Flow Package by setting LAYCON equal to 0 for all layers or in the Layer-Property Flow Package by setting LAYTYP equal to 0 for all layers), and formulations must not change based on head (such as seepage from a river changing from head dependent flow to a constant flow when head drops below the bottom of the riverbed). Examples of coefficients of simulated head for stress terms are riverbed conductance, drain conductance, maximum evapotranspiration rate, evapotranspiration extinction depth, and general-head boundary conductance.

IFREQ = 2 indicates that the flow equations are linear, but coefficients of simulated head for some stress terms may change at the start of each stress period. (See IFREQ = 1 for information about linear equations.) Examples of coefficients of simulated head for stress terms are riverbed conductance, drain conductance, maximum evapotranspiration rate, evapotranspiration extinction depth, and general-head boundary conductance. For a simulation consisting of only one stress period, IFREQ = 2 has the same meaning as IFREQ = 1.

IFREQ = 3 indicates that a nonlinear flow equation is being solved, which means that some terms in [A] depend on simulated head. Examples of head-dependent terms in [A] are transmissivity for water-table layers, where transmissivity is based on saturated thickness; flow terms for rivers, drains, and evapotranspiration if they convert between head dependent flow and constant flow; and the change in storage coefficient when a cell converts between confined and unconfined. When a nonlinear flow equation is being solved, external iteration (ITMX > 1) normally is required to accurately approximate the nonlinearities. Note that when nonlinearities caused by water-table calculations are part of a simulation, obvious signs are not necessarily produced in the output from a simulation that does not use external iteration to indicate that iteration is needed. In particular, the budget error may be acceptably small without iteration even though appreciable error exists in head because of nonlinearity. To understand this, consider the water-table correction for transmissivity. Each iteration a new transmissivity is calculated based on the previous head. Then the flow equations are solved, and a budget is computed using the new head with the same transmissivities. No appreciable budget discrepancy results because heads are correct for the transmissivity being used at this point; however, the new heads may mean that an appreciable change in transmissivity has occurred. The new transmissivity will not be calculated unless there is another iteration. Therefore, when one or more layers are under water-table conditions, iteration always should be tried. The maximum change in head in each iteration (printed by DE4 when IPRD4 = 1 and MUTD4 = 0) provides an indication of the effect of all nonlinearities.

HCLOSE is the head change closure criterion. If iterating (ITMX > 1), iteration stops when the absolute value of head change at every node is less than or equal to HCLOSE. HCLOSE is not used if not iterating, but a value always must be specified.

ACCL is a multiplier for the computed head change for each iteration. Normally, this value is 1. A value greater than 1 may be useful for improving the rate of convergence when using external iteration to solve nonlinear problems (IFREQ = 3). ACCL always should be 1 for linear problems. When ITMX = 1, ACCL is changed to 1 regardless of the input value; however, a value always must be specified.

IPRD4 is the time-step interval for printing out convergence information when iterating (ITMX > 1). For example, if IPRD4 is 2, convergence information is printed every other time step. A value always must be specified even if not iterating.

MUTD4 is a flag that indicates the quantity of information that is printed when convergence information is printed for a time step.

MUTD4 = 0 indicates that the number of iterations in the time step and the maximum head change are printed after each iteration.
MUTD4 = 1 indicates that only the number of iterations in the time step is printed.
MUTD4 = 2 indicates no information is printed.

MXUP is the maximum number of equations in the upper part of the equations to be solved (Harbaugh, 1995). This value affects the amount of memory used by the DE4 Package. If specified as 0, the program will calculate MXUP as half the number of cells in the model, which is an upper limit. The actual number of equations in the upper part will be less than half the number of cells whenever no-flow and constant-head cells exist because flow equations are not formulated for these cells. The actual number of equations in the upper part is printed when the DE4 Package runs. The printed value can be used for MXUP in future runs to minimize memory usage.

MXLOW is the maximum number of equations in the lower part of equations to be solved (Harbaugh, 1995). This value affects the amount of memory used by the DE4 Package. If specified as 0, the program will calculate MXLOW as half the number of cells in the model, which is an upper limit. The actual number of equations in the lower part will be less than half the number of cells whenever no-flow and constant-head cells exist because flow equations are not formulated for these cells. The actual number of equations in the lower part is printed when the DE4 Package runs. The printed value can be used for MXLOW in future runs to minimize memory usage.

MXBW is the maximum band width plus 1 of the [AL] matrix (Harbaugh, 1995). This value affects the amount of memory used by the DE4 Package. If specified as 0, the program will calculate MXBW as the product of the two smallest grid dimensions plus 1, which is an upper limit. The actual band width plus 1 is printed when the DE4 Package runs. The printed value can be used for MXBW in future runs to minimize memory usage.

STOR1 is a variable controlling the amount of storage allocated in the Z array for the array A and the amount of storage allocated in the IX array for the array JA. For most problems, a value of 3.0 should be adequate. If the specified value is inadequate, the output listing will indicate that the value must be increased.

STOR2 is a variable controlling the amount of storage allocated in the Z array for the arrays U and FRHS and the amount of storage allocated in the IX array for the array IA. For most problems, a value of 2.2 should be adequate. If the specified value is inadequate, the output listing will indicate that the value must be increased.

STOR3 is a variable controlling the amount of storage allocated in the IX array for the array IG. For most problems, a value of 5.4 should be adequate. If the specified value is inadequate, the output listing will indicate that the value must be increased.

ICG is a variable controlling whether or not conjugate gradient iterations are used at the end of each multigrid cycle. A value of 1 indicates that conjugate gradient iterations will be performed, whereas a value of 0 indicates no conjugate gradient iterations will be performed. All other values automatically are reset to 0. For some problems, using conjugate gradient iterations can improve convergence but also will increase the memory used by the solver.

MXITER is the maximum number of iterations—that is, calls to the AMG solver. For linear problems, MXITER can be set equal to 2. For nonlinear problems, MXITER generally needs to be larger, but rarely more than 50.

MXCYC is the maximum number of cycles allowed per call to the solver. This variable is similar to the variable ITER1 in PCG2. A value of 50 is suggested. For some nonlinear problems, however, faster convergence may be achieved by reducing MXCYC and increasing MXITER.

BCLOSE is the budget closure criterion for the scaled L2 norm of the matrix equations. A value similar to RCLOSE of PCG2 should be used. If the user desires a smaller budget error, reduce BCLOSE. Reducing BCLOSE by one order of magnitude commonly reduces the global budget error by about one order of magnitude.

DAMP is a damping/accelerating parameter identical to ACCL of the DE4 solver. Generally, a value of 1.0 is sufficient for most problems. However, for nonlinear problems, values less than 1.0 may be necessary to achieve convergence.

DAMP > 0 This value of DAMP is applied for all iterations.
DAMP = -1 Cooley's method for adaptive damping is implemented (Mehl and Hill, 2001).
DAMP = -2 The relative reduced residual method for adaptive damping is implemented.
All other values of DAMP automatically are reset to 1.0 (no damping).

IOUTAMG is a flag that controls the information printed each time step from the solver to the MODFLOW-2000 LIST output file. Diagnostic messages from the solver are sent to a temporary file called "lmg_err.tmp" except if IOUTAMG=3, when they are printed along with the other iteration information. The "lmg_err.tmp" file is deleted upon successful termination of the solver. If the solver should fail, the output in this file may help to identify solver problems. The possible values of IOUTAMG and the information printed to the LIST file are as follows:

IOUTAMG = 0 No printing from the solver to the LIST file.
IOUTAMG = 1 Print scaling for residuals and residuals before and after cycling.

IOUTAMG = 2 Print scaling for residuals, residuals before and after cycling, the computer storage used, and the computation times if the CTIME subroutine has been adapted to the computer operating system.
IOUTAMG = 3 Print solver messages, scaling for residuals, residuals after each cycle the computer storage used, and the computation times if the CTIME subroutine has been adapted to the computer operating system.

DUP is the maximum value of DAMP that should be applied at any iteration. If the adaptive scheme calculates a value of DAMP that is greater than DUP, DAMP will be reset to DUP. A value of 1.0 is reasonable for most problems.

DLOW is the minimum value of DAMP that should be applied at any iteration. If the adaptive scheme determines that the value of DAMP should be decreased, the adaptive scheme will calculate a new value of DAMP based on DLOW being the minimum. A value of 0.2 is reasonable for most problems.

OUTPUT

The OUTPUT Option (Output Control in MODFLOW) controls the amount of output from MODFLOW. If this option is not used, then default output control is used. Under the default, head and overall budget are written to the listing file (printed) at the end of every stress period. The default printout format for head and drawdown is 10G11.4.

Output File Names and Formats

"Head Print Format" and "Drawdown Print Format" are codes indicating the format for printing head and drawdown, respectively, in the LIST file (variables IHEDFM and IDDNFM). The codes are as follows:

0 - 10G11.4	11 - 20F5.4
1 - 11G10.3	12 - 10G11.4
2 - 9G13.6	13 - 10F6.0
3 - 15F7.1	14 - 10F6.1
4 - 15F7.2	15 - 10F6.2
5 - 15F7.3	16 - 10F6.3
6 - 15F7.4	17 - 10F6.4
7 - 20F5.0	18 - 10F6.5
8 - 20F5.1	19 - 5G12.5
9 - 20F5.2	20 - 6G11.4
10 - 20F5.3	21 - 7G9.2

Further, if the print code is negative, the data are printed in strip format as opposed to wrap format.

"Head Save File", "Drawdown Save File", and "IBOUND Save File" are for specifying the names of files for saving head, drawdown, and IBOUND, respectively. The data only will be saved, however, if the times for saving the data are specified in the other options of Output Control shown below. This screen also includes other options for controlling data formats:

"BINARY" and "ASCII" options—a binary file is written as a nontext file that cannot be read by a typical text editor. These files must be read by special programs that are designed to read MODFLOW's binary (unformatted) data. An ASCII file is a text file that can be read with a typical text editor.

The "Format" field specifies the format for writing an ASCII (text) file. These formats must adhere to Fortran standards, which includes a requirement to enclose the format in parentheses.

"Unlabeled" and "Labeled" options—these are options for an ASCII file. Unlabeled means the data are written without a label specifying the array name and other information such as simulation time. Labeled means there is a one-line label.

Cell-by-Cell Budget Files
The "Compact" and "Original" radio buttons determine the budget file format. Original is the original format used for MODFLOW. Compact is an optional format in MODFLOW-2000 that stores data using less disk space.

"All Data to One File" and "Specify File for Each Package" radio buttons control which files are used for saving budget data. "All Data to One File" indicates that all budget terms are written into the same file, and that file is specified in the "Name" field. "Specify File for Each Package" means that for each package that can save budget data, a file name for saving the data can be entered into the table. If the name is blank, no budget data are written for that package. If the file name is "PRINT" for WEL, RIV, GHB, DRN, BCF, or LPF, then budget data are written to the listing file.

Times for Printing Head
This option allows the times for printing head in the LIST file to be specified. The options are "None", "Simulation End", "Every Stress Period", "All Time Steps", and "List". The first four of these options require no additional input. The "List" option requires the user to specify a list of stress periods and time steps at which head should be printed.

Times for Saving Head
This option allows the times for saving head to be specified. The options are the same as for printing head. Note that head will not be saved unless a file name is specified using the "Output File Names" option above.

Times for Printing Drawdown
This option allows the times for printing drawdown in the LIST file to be specified. The options are the same as for printing head.

Times for Saving Drawdown
This option allows the times for saving drawdown to be specified. The options are the same as for printing head. Note that drawdown will not be saved unless a file name is specified using the "Output File Names" option above.

Times for Printing Budget
This option allows the times for printing the overall budget in the LIST file to be specified. The options are the same as for printing head, except that "None" and "Simulation End" cannot be selected because the budget must be printed at least at the end of every stress period.

Times for Saving Flow (CBC) Data
This option allows the times for saving budget data to be specified. The options are the same as for printing head. Note that budget data will not be saved unless a file name (or names) is specified using the "Output File Names" option above.

Times for Saving IBOUND
This option allows the times for saving IBOUND to be specified. The options are the same as for printing head. Note that IBOUND will not be saved unless a file name is specified using the "Output File Names" option above.

Comments
Comments are placed at the beginning of the Output Control file.

MODPATH

Prepare data for running MODPATH.

Check
This option checks the MODPATH data to determine whether data are complete. If not complete, the incomplete data are listed.

Misc.
Maximum number of particles—Specify 0 to use the default incorporated in MODPATH.

Maximum size of composite budget file—This value is used only for transient simulations. Specify 0 to use the default maximum file size. If the maximum is exceeded, MODPATH prompts the user to determine if it is OK to exceed that size.

Output style—MODPATH can save data in various formats, and this option allows the format to be chosen.

Modpath-Plot Water Table—Modpath-Plot can draw the water table using various line types, and this option allows the line type to be chosen.

Time assigned to the beginning of the MODFLOW simulation

Time range for data in budget file—To save disk space in transient simulations, MODFLOW requires only that budget data generated by MODFLOW be saved for the duration of time for which particles are tracked.

IBOUND
MODPATH includes an IBOUND variable that is similar to MODFLOW's IBOUND. One value is read for every model cell. In addition to indicating variable head (> 0), no flow (= 0), and constant head (< 0), specific positive IBOUND values are used in MODPATH to indicate plotting colors and areas for stopping particles. The following editing options allow the MODPATH IBOUND values to be defined for each layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the MODPATH MAIN data file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

When MODPATH is first activated in MFI2K, MODFLOW IBOUND values are used as initial values for MODPATH IBOUND if the Constant or Package options are used for MODFLOW.

Porosity
Darcy velocity is divided by porosity to obtain actual velocity. The following editing options allow the porosity values to be defined for each layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the MODPATH MAIN data file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

GUA Method
Specifies how the Grid Unit Array (GUA) is used when plotting.

- None—GUA is not used.
- ZONES—The GUA is an Integer array, and the value at each cell determines the color of the cell when the GUA is plotted.
- Nonuniform RANGES—The GUA is a Real array. A table of arbitrary numeric ranges is defined, and each range is assigned a number. The color plotted is determined from the range number to which the GUA value corresponds.

- Uniform RANGES—The GUA is a Real array. A table of numeric ranges with a uniform interval is defined, and each range is assigned a number. The color plotted is determined from the range number to which the GUA value corresponds.

Grid Unit Array

The following editing options allow the GUA to be defined for each layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the MODPATH MAIN data file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

GWT

Prepare data for the Ground-Water Transport Process. When this menu item initially is activated in MFI2K, a screen for specifying the transport subgrid appears. Subsequent use of this menu item will not cause the subgrid screen to appear.

Check Complete

This option checks the GWT data to determine whether data are complete. If not complete, the incomplete data are listed.

Miscellaneous

The need for some of these variables depends on the transport method—MOC, MOCMP, or ELLAM—specified in the GWT dialog. Unneeded fields cannot be modified.

HEDMOC is the GWT simulation title.

CNOFLO is the concentration associated with inactive cells of subgrid (used for output purposes only).

DECAY is the first-order decay rate [1/T] (DECAY = 0 indicates that no decay occurs).

DIFFUS is the effective molecular diffusion coefficient [L^2/T]

CELDIS is the maximum fraction of cell dimension that a particle may move in one time step (typically, $0.5 \leq FZERO \leq 0.05$).

NPMAX is the maximum number of particles available for particle tracking of advective transport. If set to 0, the model will calculate NPMAX according to the following equation:

NPMAX = 2*NPTPND*NSROW*NSCOL*NSLAY

NPTPND is the initial number of particles per cell in transport simulation (that is, at t = 0.0). Valid options for default geometry of particle placement include 1, 2, 3, or 4 for 1-D transport; 1, 4, 9, or 16 for 2-D transport; and 1, 8, or 27 for 3-D transport. The user also can customize initial placement of particles by specifying NPTPND as a negative number, in which case the minus sign is recognized as a flag to indicate custom placement as desired. In this case, the subsequent screen will prompt for values of PNEWL, PNEWR, and PNEWC for each particle. These values are the relative positions in the layer, row, and column, respectively, for initial placement of the particle within any finite-difference cell.

FZERO is a fractional value. If the fraction of active cells having no particles exceeds FZERO, the program automatically will regenerate an initial particle distribution before continuing the simulation (typically $0.01 \leq FZERO \leq 0.05$).

INTRPL is the interpolation scheme—choose linear or bilinear.

FDTMTH is the weighting factor for temporal differencing of the dispersion equation ($0.0 \leq$ FDTMTH ≤ 1.0). We suggest using either FDTMTH = 0.5, a centered-in-time (or Crank-Nicolson) approximation, or FDTMTH = 1.0, a backward-in-time (or fully implicit) approximation.

NCXIT is the number of iterations for the explicitly lagged, cross-dispersive flux terms (NCXIT ≥ 1). The user is advised to initially specify a value of 2, but if the solution exhibits large areas of negative concentrations, then the value of NCXIT should be increased to require more iterations, which typically will reduce the extent and magnitude of negative concentrations.

IDIREC is the direction index for permutation of the red-black node renumbering scheme. The order is as follows: 1: x,y,z; 2: x,z,y; 3: y,x,z; 4: y,z,x; 5: z,x,y; and 6: z,y,x. The first direction index is advanced least rapidly. The user is advised to initially specify IDIREC = 1. If this leads to a relatively large number of iterations (more than 10), then the user should experiment with alternate choices.

EPSSLV is the tolerance on the relative residual for the conjugate-gradient solution of the matrix of the difference equations. The user initially should specify EPSSLV $\leq 10^{-5}$.

MAXIT is the maximum number of iterations allowed for the iterative solution to the different equations for dispersive transport. In most cases, MAXIT = 100 is satisfactory.

NSCEXP is the exponent used to calculate the number of subcells in the column direction (NSC, where NSC = 2**NSCEXP) when ELLAM is used.

NSREXP is the exponent used to calculate the number of subcells in the row direction (NSR) when ELLAM is used.

NSLEXP is the exponent used to calculate the number of subcells in the layer direction (NSL) when ELLAM is used.

NTEXP is the exponent used to calculate the number of sub-time steps per transport time increment (NT) when ELLAM is used.

Initial Concentration

Define values for the initial concentration for the subgrid. The following editing options allow the values to be defined for each subgrid layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the GWT file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Concentration Outside the Subgrid

Define concentration outside of the subgrid. One value is required for each layer of the full MODFLOW grid that has interaction with a GWT subgrid layer.

Fixed-Head Concentration Zones

Define a table of zone numbers (IZONE) and corresponding source concentration (ZONCON). The source concentrations apply to constant-head cells. The ZONCON concentration value is applied to all cells that have an IBOUND value (BAS Package) equal to the IZONE value. IZONE values must be negative because IBOUND is negative at constant-head cells. A concentration of 0.0 is used for constant-head cells where there is no corresponding IZONE value.

Strong Source Flags

Define strong source flags for the subgrid. The following editing options allow the values to be defined for each subgrid layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the GWT file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Retardation

Define retardation factor (RF) values for the subgrid. The following editing options allow a single one-dimensional array to be defined that has one value for each GWT subgrid layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the GWT file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Porosity

Define porosity for the subgrid. The following editing options allow the values to be defined for each subgrid layer:

- Constant—all elements of the array have the same value.
- Package—data are saved in the GWT file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Recharge Concentration

Define values for the recharge concentration for the subgrid. The following editing options allow a subgrid layer array to be defined for each stress period:

- Constant—all elements of the array have the same value.
- Package—data are saved in the GWT file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Output

This screen controls the output of four kinds of data for the GWT Process: Concentration, Velocity, Dispersion, and Particles. To activate output of the different types, the output frequency must be specified. The Output Interval can be End of Simulation, Every Period, Every Time Step, or Time-Step Interval. If Time-Step Interval is specified, an Integer value is specified for the interval. For example, if the interval is 5, then output occurs every 5 time steps. For all the output types except dispersion, an output file name must be specified (ASCII or Binary). The ASCII name can be the LIST file. Dispersion output can go only to the listing file.

Conc. Observations

Defines a table of cell locations for which simulated concentration will be written.

Transport Solution Method

Specifies the transport method – MOC, MOCMP, or ELLAM.

Dispersion

Specifies if dispersion is on or off. If on, values of Longitudinal, Horizontal Transverse, and Vertical Transverse dispersion must be specified. Each of these is a one-dimensional array with one value for each GWT subgrid layer. The following editing options allow each dispersion array to be defined:

- Constant—all elements of the array have the same value.

- Package—data are saved in the GWT file, and the external editing mechanism is used to modify the data.
- Separate—data are stored in a separate file that MFI2K does not read.

Observations

All Observations

OUTNAM indicates whether or not a variety of output files are produced. If "NONE" is specified, none of the output files are generated. Otherwise, the output files are named using OUTNAM as the base followed by a period and a two- or three-character extension.

ISCALS is a flag for controlling the printing of the observation-sensitivity tables.

- None—No observation-sensitivity tables are printed, but a table showing composite scaled sensitivity for each parameter is printed.
- Unscaled sensitivities—Unscaled sensitivities are printed.
- Dimensionless scaled sensitivities—Dimensionless scaled sensitivities are printed. Sensitivities are scaled by multiplying by the parameter value and the square root of the weight, which produces dimensionless numbers.
- 1% sensitivities—One-percent sensitivities are printed. Sensitivities are scaled by multiplying the unscaled sensitivities by the parameter value and dividing by 100.
- Dimensionless and 1% sensitivities—Both dimensionless scaled and 1% sensitivities are printed.

Sngl. Time Head

This option allows head observations for single times to be specified. Two variables, a table, and two special pushbuttons are displayed.

Variables:

TOMULTH is the time-offset multiplier for head observations. The product of TOMULTH and TOFFSET must produce a time value in the units used for all other model input data. The same variable appears in the Multi-Time Head screen.

EVH is the input error variance multiplier for hydraulic-head observations. EVH is used to calculate the weights in the calculation of STATISTIC. The same variable appears in the Multi-Time Head screen.

Table:

Each row in the table can contain one observation; the fields in the table are described below. Rows in which the "Obs. Name" field is blank are ignored.

Obs. Name is a string of 1 to 12 nonblank characters used to identify the observation.

Layer is the layer in which the observation is located. If an observation is for a single layer, the layer can be edited directly in the table. If an observation is multilayer, the layer field is disabled, and the Edit Multilayer pushbutton must be used to specify the layers.

Row is the row in which the observation is located.

Column is the column in which the observation is located.

IREFSP is the stress period to which the observation time (TOFFSET) is referenced. The reference point is the beginning of stress period IREFSP.

TOFFSET is the time from the beginning of stress period IREFSP to the time of the observation.

HOBS is the observed head.

STATISTIC is the value from which the observation weight is calculated.

STAT-FLAG is a flag identifying the type of statistic specified in STATISTIC:
Variance—scaled variance.
Stnd. Dev. —scaled standard deviation.
Coef. of Var. —scaled coefficient of variation.

ROFF is the row offset used to locate the observation in the finite-difference cell. For an observation in row i, 0.0 is the center of the cell, -0.5 is the face between rows i-1 and i, and +0.5 is the face between rows i and i+1.

COFF is the column offset used to locate the observation in the finite-difference cell. For an observation in column j, 0.0 is the center of the cell, -0.5 is the face between columns j-1 and j, and +0.5 is the face between columns j and j+1.

Pl. Sy. is an integer that is written to output files intended for graphical analysis to allow control of the symbols used to plot data.

Pushbuttons:

Edit Multilayer—allows multiple model layers to be assigned to observations. Additional dialogs allow an observation to be selected and the layers to which the observation corresponds to be specified. For each layer, the proportion of the simulated head that is used to calculate the simulated multilayer head also is specified.

Comments—allows comments to be included in the head observations file.

Multi-Time Head

This option allows head observations for multiple times at the same location to be specified. Two variables, a table, and three special pushbuttons are displayed.

Variables:

TOMULTH is the time-offset multiplier for head observations. The product of TOMULTH and TOFFSET must produce a time value in the units used for all other model input data. The same variable appears in the Sngl. Time Head screen.

EVH is the input error variance multiplier for hydraulic-head observations. EVH is used to calculate the weights in the calculation of STATISTIC. The same variable appears in the Sngl. Time Head screen.

Table:

Each row in the table shows a summary of information for one location with mult-time observations.

Pushbuttons:

Comments—allows comments to be included in the head observations file.

New Multi-Time Observation—allows a new location at which multi-time observations can be specified. This starts another dialog that allows the observation to be defined. The additional dialog is the same as the dialog for the following pushbutton.

Edit Multi-Time Observation—allows the selected observation to be modified using a separate dialog. There are five individual fields, radio buttons, and two tables in the dialog:

Multi-Time Observation Fields:

Header Name is a string of 1 to 12 nonblank characters used to identify the observation.

Row is the row in which the observation is located.

Column is the column in which the observation is located.

Row Offset (variable ROFF) is used to locate the observation in the finite-difference cell. For an observation in row i, 0.0 is the center of the cell, -0.5 is the face between rows i-1 and i, and +0.5 is the face between rows i and i+1.

Column Offset (variable COFF) is used to locate the observation in the finite-difference cell. For an observation in column j, 0.0 is the center of the cell, -0.5 is the face between columns j-1 and j, and +0.5 is the face between columns j and j+1.

Radio Buttons:

Use the buttons to specify whether the objective function is based on head or drawdown.

First Table:

Layer is the layer in which the observation applies. If there are multiple rows in which Layer > 0, the observation is multi-layer.

Proportion is the proportion of the simulated head that is used to calculate the simulated multilayer head. If there is only one row in which Layer > 0, proportion is not used.

Second Table:

Name is a string of 1 to 12 nonblank characters used to identify the observation.

IREFSP is the stress period to which the observation time (TOFFSET) is referenced. The reference point is the beginning of stress period IREFSP.

TOFFSET is the time from the beginning of stress period IREFSP to the time of the observation.

HOBS is the observed head.

STATh is the value from which the observation weight is calculated if the objective function is based on head.

STATdd is the value from which the observation weight is calculated if the objective function is based on drawdown.

STAT-FLAG is a flag identifying the type of statistic specified in STATh or STATdd (whichever is used):
Variance—scaled variance.
Stnd. Dev. —scaled standard deviation.
Coef. of Var. —scaled coefficient of variation.

Pl. Sy. is an integer that is written to output files intended for graphical analysis to allow control of the symbols used to plot data.

GHB Observations

Time offset multiplier (variable TOMULTGB)—The product of TOMULTGB and TOFFSET (in the observation time dialog) must produce a time value in the units used for all other model input data.

Error variance for observations (variable EVFGB) —EVFGB is used to calculate the weights in the calculation of STATISTIC (in the observation time dialog).

The list shows all of the observation groups that have been defined.

"DELETE Cell group" causes the selected group to be deleted.

"ADD Cell group" causes a new observation group to be created with 0 times and locations.

"EDIT Observation Times" allows observed values to be specified for multiple times. A separate screen with the following fields is activated:

OBSNAM is a string of 1 to 12 nonblank characters used to identify the observation.

IREFSP is the stress period to which the observation time (TOFFSET) is referenced. The reference point is the beginning of stress period IREFSP.

TOFFSET is the time from the beginning of stress period IREFSP to the time of the observation.

HOBS is the observed inflow to the ground-water system from the boundary (negative indicates outflow).

STATISTIC is the value from which the observation weight is calculated.

STAT-FLAG is a flag identifying the type of statistic specified in STATISTIC:
Variance—scaled variance.
Stnd. Dev.—scaled standard deviation.
Coef. of Var.—scaled coefficient of variation.

Pl. Sy. is an integer that is written to output files intended for graphical analysis to allow control of the symbols used to plot data.

"EDIT Cell Locations" allows the cells that define the location of the observation to be specified. A separate screen with the following fields is activated:

Layer is the layer number of a boundary cell that is in the cell group.

Row is the row number of a boundary cell that is in the cell group.

Column is the column number of a boundary cell that is in the cell group.

FACTOR is the portion of the simulated flow for this cell that is included in the total simulated flow for this cell group.

"Force Factor=1.0 for all cells" is a check box that causes FACTOR to be set to 1.0 for all cells in the cell group when MODLFOW runs regardless of the values for FACTOR in the table.

DRN Observations

Time offset multiplier (variable TOMULTDR)—The product of TOMULTDR and TOFFSET (in the observation time dialog) must produce a time value in the units used for all other model input data.

Error variance for observations (variable EVFDR) —EVFDR is used to calculate the weights in the calculation of STATISTIC (in the observation time dialog).

The list shows all of the observation groups that have been defined.

"DELETE Cell group" causes the selected group to be deleted.

"ADD Cell group" causes a new observation group to be created with 0 times and locations.

"EDIT Observation Times" allows observed values to be specified for multiple times. A separate screen with the following fields is activated:

OBSNAM is a string of 1 to 12 nonblank characters used to identify the observation.

IREFSP is the stress period to which the observation time (TOFFSET) is referenced. The reference point is the beginning of stress period IREFSP.

TOFFSET is the time from the beginning of stress period IREFSP to the time of the observation.

HOBS is the observed inflow to the ground-water system from the boundary (negative indicates outflow). The value must be negative for the Drain Package.

STATISTIC is the value from which the observation weight is calculated.

STAT-FLAG is a flag identifying the type of statistic specified in STATISTIC:
Variance—scaled variance.

Stnd. Dev.—scaled standard deviation.
Coef. of Var.—scaled coefficient of variation.

Pl. Sy. is an integer that is written to output files intended for graphical analysis to allow control of the symbols used to plot data.

"EDIT Cell Locations" allows the cells that define the location of the observation to be specified. A separate screen with the following fields is activated:

Layer is the layer number of a drain cell that is in the cell group.

Row is the row number of a drain cell that is in the cell group.

Column is the column number of a drain cell that is in the cell group.

FACTOR is the portion of the simulated flow for this cell that is included in the total simulated flow for this cell group.

"Force Factor = 1.0 for all cells" is a check box that causes FACTOR to be set to 1.0 for all cells in the cell group when MODLFOW runs regardless of the values for FACTOR in the table.

RIV Observations

Time offset multiplier (variable TOMULTRV)—The product of TOMULTRV and TOFFSET (in the observation time dialog) must produce a time value in the units used for all other model input data.

Error variance for observations (variable EVFRV)—EVFRV is used to calculate the weights in the calculation of STATISTIC (in the observation time dialog).

The list shows all of the observation groups that have been defined.

"DELETE Cell group" causes the selected group to be deleted.

"ADD Cell group" causes a new observation group to be created with 0 times and locations.

"EDIT Observation Times" allows observed values to be specified for multiple times. A separate screen with the following fields is activated:

OBSNAM is a string of 1 to 12 nonblank characters used to identify the observation.

IREFSP is the stress period to which the observation time (TOFFSET) is referenced. The reference point is the beginning of stress period IREFSP.

TOFFSET is the time from the beginning of stress period IREFSP to the time of the observation.

HOBS is the observed inflow to the ground-water system from the river (negative indicates outflow).

STATISTIC is the value from which the observation weight is calculated.

STAT-FLAG is a flag identifying the type of statistic specified in STATISTIC:
Variance—scaled variance.
Stnd. Dev.—scaled standard deviation.
Coef. of Var.—scaled coefficient of variation.

Pl. Sy. is an integer that is written to output files intended for graphical analysis to allow control of the symbols used to plot data.

"EDIT Cell Locations" allows the cells that define the location of the observation to be specified. A separate screen with the following fields is activated:

Layer is the layer number of a river cell that is in the cell group.

Row is the row number of a river cell that is in the cell group.

Column is the column number of a river cell that is in the cell group.

FACTOR is the portion of the simulated flow for this cell that is included in the total simulated flow for this cell group.

"Force Factor = 1.0 for all cells" is a check box that causes FACTOR to be set to 1.0 for all cells in the cell group when MODLFOW runs regardless of the values for FACTOR in the table.

Constant-head Obs.

Time offset multiplier (variable TOMULTCH)—The product of TOMULTCH and TOFFSET (in the observation time dialog) must produce a time value in the units used for all other model input.

Error variance for observations (variable EVFCH) —EVFCH is used to calculate the weights in the calculation of STATISTIC (in the observation time dialog).

The list shows all of the observation groups that have been defined.

"DELETE Cell group" causes the selected group to be deleted.

"ADD Cell group" causes a new observation group to be created with 0 times and locations.

"EDIT Observation Times" allows observed values to be specified for multiple times. A separate screen with the following fields is activated:

OBSNAM is a string of 1 to 12 nonblank characters used to identify the observation.

IREFSP is the stress period to which the observation time (TOFFSET) is referenced. The reference point is the beginning of stress period IREFSP.

TOFFSET is the time from the beginning of stress period IREFSP to the time of the observation.

HOBS is the observed inflow to the ground-water system from the boundary (negative indicates outflow).

STATISTIC is the value from which the observation weight is calculated.

STAT-FLAG is a flag identifying the type of statistic specified in STATISTIC:
Variance—scaled variance.

Stnd. Dev.—scaled standard deviation.
Coef. of Var.—scaled coefficient of variation.

Pl. Sy. is an integer that is written to output files intended for graphical analysis to allow control of the symbols used to plot data.

"EDIT Cell Locations" allows the cells that define the location of the observation to be specified. A separate screen with the following fields is activated:

Layer is the layer number of a boundary cell that is in the cell group.

Row is the row number of a boundary cell that is in the cell group.

Column is the column number of a boundary cell that is in the cell group.

FACTOR is the portion of the simulated flow for this cell that is included in the total simulated flow for this cell group.

"Force Factor=1.0 for all cells" is a check box that causes FACTOR to be set to 1.0 for all cells in the cell group when MODLFOW runs regardless of the values for FACTOR in the table.

Sensitivity

The Sensitivity screen allows the Sensitivity Process to be controlled. A variable, a pushbutton, and a table are displayed.

Variables:

ISENALL is a flag that can override values of ISENS in the table below and can deactivate parameter estimation:

- Use ISENS flags to determine if sensitivity and parameter values will be calculated.
- Calculate sensitivity for all parameters in sensitivity file (but turn off parameter estimation).
- Do not calculate sensitivity and turn off parameter estimation. This option causes a forward flow simulation to use the parameter values in the Sensitivity file rather than the values specified as part of the parameter definitions.

IPRINTS is a flag indicating whether the OUTPUT Control head print flag controls the output of the sensitivity arrays. This flag has meaning only if a sensitivity save file or print file is specified:

Yes—The sensitivity arrays are output whenever the head print flag in Output Control is set. The layers of output also are limited to the layers for which head is printed.
No—The sensitivity arrays are output every time step, and all layers are output.

Sensitivity Save File—The name of the file to which sensitivity arrays will be saved. MFI2K assigns a file unit number to this file, which is input variable ISENSU in the SEN input file.

Sensitivity Print File—The name of the file to which sensitivity arrays will be printed. This file can be the name of the GLOBAL file, the LIST file, or another file that is not used elsewhere. MFI2K assigns a file unit number to this file, which is input variable ISENPU in the SEN input file.

ISENFM is the print code for printing sensitivity arrays in the sensitivity print file. The allowed codes are:

0 - 10G11.4 11 - 20F5.4
1 - 11G10.3 12 - 10G11.4

2 - 9G13.6 13 - 10F6.0
3 - 15F7.1 14 - 10F6.1
4 - 15F7.2 15 - 10F6.2
5 - 15F7.3 16 - 10F6.3
6 - 15F7.4 17 - 10F6.4
7 - 20F5.0 18 - 10F6.5
8 - 20F5.1 19 - 5G12.5
9 - 20F5.2 20 - 6G11.4
10 - 20F5.3 21 - 7G9.2

If a negative value is specified, the sensitivity arrays are not printed.

Pushbutton:

"Select Parameters to be Included in SEN File" allows any currently defined parameter to be included in the SEN File.

Table:

The table contains the following fields for each parameter that will be included in the SEN File:

Name (variable PARNAM in the MODFLOW documentation) is the name of a previously defined parameter. This field cannot be modified.

ISENS is a check box field that indicates whether sensitivity of the parameter will be calculated. If the Parameter-Estimation Process is active, this value also determines whether the parameter value will be estimated.

Log Transform (variable LN in the MODFLOW documentation) is a check box field that indicates whether the parameter is log-transformed for parameter estimation.

SEN File Value (variable B in the MODFLOW documentation) is the starting value of the parameter. In the Sensitivity file, this value can be different from the value that is specified when the parameter is defined, and this value in the Sensitivity file is used as the starting value.

GWF File Value is the value of the parameter that is specified when the parameter is defined. This value cannot be modified in the SEN screen. If the Sensitivity Process is active, the GWF File Value is not used. It is shown in this screen for information purposes.

Min. Value (variable BL in the MODFLOW documentation) is the minimum reasonable parameter value. This value does not restrict the estimated value when parameter estimation is used. This value is printed in the model output to facilitate comparison with the estimated value.

Max. Value (variable BU in the MODFLOW documentation) is the maximum reasonable parameter value. This value does not restrict the estimated value when parameter estimation is used. This value is printed in the model output to facilitate comparison with the estimated value.

BSCAL is an alternate scaling factor for the parameter. Good choices are the minimum (in absolute value) reasonable value of the parameter or a value two or three orders of magnitude smaller than the parameter value.

Par. Est.

This screen allows the Parameter-Estimation Process to be controlled. Many variables and two lists are displayed.

Variables:

MAX-ITER is the maximum number of parameter-estimation iterations. If MAX-ITER = 0, the program calculates the variance-covariance matrix on parameters and related statistics (the parameter correlation coefficients generally are of most interest) using the starting parameter values from the Sensitivity Process input file, and parameter estimation stops after one iteration.

MAX-CHANGE is the maximum fractional change for parameter values in one iteration. MAX-CHANGE commonly equals 2.0, or less if parameter values are unstable during parameter-estimation iterations.

TOL is the parameter-estimation closure criteria, as a fractional change in parameter values. TOL commonly equals 0.01. Larger values often are used during preliminary calibration efforts; values as small as 0.001 can be used.

SOSC is the second convergence criterion. If SOSC $\neq$ 0.0, parameter estimation will converge if the least-squares objective function does not decrease by more than SOSC$\times$100 percent over two parameter-estimation iterations. SOSC usually equals 0.0. Typical nonzero values of SOSC are 0.01 and 0.05.

IBEFLG is a flag that controls the generation of files to be used as input to the post-processing program BEALE-2000, which tests model linearity:

IBEFLG = 0, no file for BEALE-2000 is produced.
IBEFLG = 1, the _b1 file is produced.
IBEFLG = 2, the _b2 file is produced. Production of this file may require MODFLOW-2000 input files that differ from the files used for model calibration.

IYCFLG is a flag that controls the generation of files to be used as input to the post-processing program YCINT-2000, which calculates confidence and prediction intervals on simulated equivalents to observations:

- IYCFLG = 0, The _y0 file is produced. Production of this file may require MODFLOW-2000 input files that differ from the files used for model calibration.
- IYCFLG = 1, The _y1 file is produced. Production of this file may require MODFLOW-2000 input files that differ from the files used for model calibration. Sensitivities for the predicted quantities are calculated, but the calculations related to nonlinear regression and the variance-covariance matrix on parameters are not made.
- IYCFLG = 2, The _y2 file is produced. This file is needed if confidence and prediction intervals on differences are to be calculated. Production of this file may require MODFLOW-2000 input files that differ from the files used for model calibration. Sensitivities for the predicted quantities are calculated, but the calculations related to nonlinear regression and the variance-covariance matrix on parameters are not made.

IOSTAR is a flag that controls printing to the screen. If IOSTAR = 1, printing to the screen is suppressed; usually IOSTAR = 0.

NOPT is a flag identifying whether or not to include matrix $\underline{R}$ of equation (B1) in equation (4a), as described in Hill (1998, p. 8, 78). Regression may converge in fewer iterations with NOPT = 1 for problems with large residuals and a large degree of nonlinearity.

NFIT is the number of Gauss-Newton iterations (when NOPT equals 1) after which matrix $\underline{R}$ of equation (B1) is included in equation (4a) of Hill (1998, p. 8, 79).

SOSR is a criterion for using R of equation (B1) in equation (4a) of Hill (1998, p. 8,78). Matrix R is used if the percentage change in the sum of squared, weighted residuals does not exceed SOSR*100 in two parameter-estimation iterations. Usually SOSR equals 0.0.

RMAR is used along with RMARM to calculate the Marquardt parameter, if its use is indicated based on variable CSA (below). Typically, RMAR = 0.001.

RMARM is used along with RMAR to calculate the Marquardt parameter, if its use is indicated based on variable CSA (below). Typically, RMARM = 1.5.

IAP is a flag identifying whether, for log-transformed parameters, MAX-CHANGE applies to the native parameter value or to the log transform of the parameter value. Usually, IAP = 0.

- IAP = 0, MAX-CHANGE applies to the native parameter value.
- IAP = 1, MAX-CHANGE applies to the log transform of the parameter value.

IPRCOV is a format code for printing of variance-covariance and correlation matrices. Permissible values of IPRCOV and corresponding formats are:

IPRCOV	FORMAT	IPRCOV	FORMAT
1	11G10.3	6	6G10.3
2	10G11.4	7	5G11.4
3	9G12.5	8	5G12.5
4	8G13.6	9	4G13.6
5	8G14.7	10	4G14.7

IPRINT is a flag that controls printing of various statistics computed for each parameter-estimation iteration, including simulated equivalents, unweighted and weighted residuals, observation sensitivities, summary statistics for residuals by observation type, scaled least-squares matrix of the Gauss-Newton method, and scaled gradient vector of the objective function.

- IPRINT = 0, the statistics are printed at the first and last parameter-estimation iterations.
- IPRINT > 0, the statistics are printed at each iteration. Also, a summary of parameter values and statistics for all parameter-estimation iterations is printed in the GLOBAL output file.

LPRINT is a flag that controls printing of eigenvalues and eigenvectors.

- LPRINT = 0, eigenvalues and eigenvectors are not printed.
- LPRINT > 0, if parameter estimation converges, eigenvalues and eigenvectors are printed.

CSA is the search-direction adjustment parameter used in the Marquardt procedure. Usually CSA = 0.08.

FCONV is a flag and a value used to allow coarser solver convergence criteria for early parameter-estimation iterations. If FCONV equals 0.0, coarser convergence criteria are not used. Commonly, FCONV = 0.0; typical nonzero values are 5.0 or 10.0, and these can result in much smaller execution times in some circumstances.

LASTX is a flag that controls calculation of the sensitivities used to calculate the parameter variance-covariance matrix when parameter estimation converges.

- LASTX = 0, sensitivities from the last parameter-estimation iteration are used to calculate the variance-covariance matrix. The program proceeds as in figure 1.
- LASTX > 0, sensitivities are recalculated using the final parameter estimates and are used to calculate the variance-covariance matrix.

Lists:
PARNEG is a list of the names of parameters that can have negative values. Negative parameters are limited to types HK, VK, VANI, VKCB, SS, SY, or EVT.

Prior Information is defined in a table. Each row defines one prior information equation :

EQNAM is a user-supplied name (up to 10 nonblank characters) for a prior-information equation.

PRM is the prior estimate for prior-information equation EQNAM. PRM always needs to be specified as a native, untransformed value. That is, even if the parameter is specified as being log-transformed in the Sensitivity Process input file, here PRM needs to be the untransformed value.

"Expression for model equivalent of PRM" defines how to calculate PRM from model information. This expression has the form:

[SIGN] [COEF "*"] PNAM [SIGN [COEF "*"] PNAM [SIGN…]]

- SIGN is either "+" or "-" (entered without quotes). The SIGN before the first PARNAM is assumed to be "+", unless otherwise indicated.
- COEF is the coefficient for parameter PNAM. COEF can be specified with or without a decimal point and can be specified in scientific notation.
- "*" indicates that an asterisk (without quotes) must be entered literally if a value for COEF is entered.
- PNAM is a parameter name as specified in the SEN file. If the parameter is designated in the SEN file as being log-transformed (LN > 0), the prior-information equation may contain only one parameter name. If a prior-information equation contains no log-transformed parameters, the equation may contain any number of terms, where each term is defined by the sequence: SIGN [COEF "*"] PNAM.
- The simplest example is prior information about an individual parameter. For example, consider that the hydraulic conductivity parameter, HK1, previously has been defined in the LPF Package. The expression in this case would be simply HK1—there is no need for SIGN, COEF, or "*".

STATP is the value from which the weight for prior-information equation EQNAM is calculated, as determined using STAT-FLAG. If a parameter is specified as being log-transformed in the Sensitivity Process input file, STATP may be specified relative either to the native value or to the log-transformed value (using log base 10), depending on the value of STAT-FLAG.

STAT-FLAG is a flag identifying how the weight for prior-information equation EQNAM is to be calculated. This calculation depends both on whether the user chooses to specify the variance, standard deviation, or coefficient of variation, and whether, for log-transformed parameters, the user chooses to specify the statistic related to the native, untransformed parameter, or to the transformed parameter.

- STAT-FLAG = 0, STATP is the variance associated with PRM and is related to the native prior value. Weight = 1/STATP unless the parameter is defined as log-transformed in the Sensitivity Process input file, in which case equation 27 is used to convert STATP (which equals σ^2_b of equation 27) to $\sigma^2_{\ln b}$, and weight = $1/\sigma^2_{\ln b}$.
- STAT-FLAG = 1, STATP is the standard deviation associated with PRM, and is related to the native prior value. Weight = $1/STATP^2$ unless the parameter value is defined as log-transformed in the Sensitivity Process input file, in which case equation 27 is used to convert STATP (which equals σ_b of equation 27) to $\sigma^2_{\ln b}$ and weight = $1/\sigma^2_{\ln b}$.

- STAT-FLAG = 2, STATP is the coefficient of variation associated with PRM, and is related to the native prior value. Weight = $1/(\text{STATP} \times \text{PRM})^2$ unless the parameter is defined as log-transformed in the Sensitivity Process input file, in which case equation 27 is used to convert STATP (which equals σ_b/b of equation 27) to $\sigma^2_{\ln b}$ and weight = $1/\sigma^2_{\ln b}$.
- STAT-FLAG = 10, STATP is the variance associated with the log (base 10) transform of PRM; weight = $1/[\text{STATP} \times 2.3026^2]$.
- STAT-FLAG = 11, STATP is the standard deviation associated with the log (base 10) transform of PRM; weight = $1/[\text{STATP}^2 \times 2.3026^2]$.
- STAT-FLAG = 12, STATP is the coefficient of variation associated with the log (base 10) transform of PRM; weight = $1/[(\text{STATP} \times \log_{10}(\text{PRM}))^2 \times 2.3026^2]$.

PLOT-SYMBOL is an integer that will be written to output files intended for graphical analysis to allow control of the symbols used when plotting data related to prior information.

External Editing Mechanism

Arrays or lists that are defined using the package method will be included in the primary data file for the package or option to which the data belongs. For example, if the array of recharge rates is defined using the package method, the array will be included in the RCH file. When using MFI2K, package data can be edited using an external program such as a text editor or a spreadsheet program. The external editing mechanism is activated when an array is first specified as being defined using the package method or when the "Send for External Editing" pushbutton is selected. The external editing mechanism consists of the following steps:

1. When the mechanism is activated, MFI2K writes the current values of the array or list into a file named _mfiss.csv. This file is a comma-delimited text file.

2. MFI2K displays a message box telling the user to edit _mfiss.csv.

3. The user should not immediately respond to the message box. Rather, the user should activate the external program and edit _mfiss.csv as desired. A typical text editor, such as Notepad, can be used as the editor.

4. When done editing the data, the user must save the modified data back into _mfiss.csv using a comma-delimited structure. The fields must be separated by a comma with optional additional spaces, and each field must have a nonblank value. However, the width of each field does not have to be the same.

5. The user must then close _mfiss.csv in the external program. The external program need not be terminated provided _mfiss.csv can be closed without terminating the editing program.

6. The user should respond with OK to the MFI2K message box.

7. MFI2K will then read the modified values that were placed back into _mfiss.csv by the external program.

8. MFI2K continues processing user commands.

Instructions for using Excel as the external editing program:

Reading _mfiss.csv—Use the Open option in Excel, and select the file _mfiss.csv in the directory in which MFI2K is running.

Saving data back into _mfiss.csv—The quickest way to complete steps 4-5 above is to use the Close option in Excel without separately specifying the Save option:

1. Choose the Close option.

2. If the data have been modified, Excel always asks if the data should be saved. Respond with “Yes”.

3. The “Save As” screen then will display the file name (which should still should be _mfiss.csv). Respond with OK.

4. Respond with “Yes” to the prompt to replace the existing file.

5. Finally, Excel will inform the user that a text file cannot save all information in a spreadsheet, and will ask if the user wants to leave the file in this format. Respond with “Yes” to keep the comma-delimited text format.